USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Buch
989348

STRUCTURE FILE UPDATES: 28 APR 2002 HIGHEST RN 408492-65-9
DICTIONARY FILE UPDATES: 28 APR 2002 HIGHEST RN 408492-65-9

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

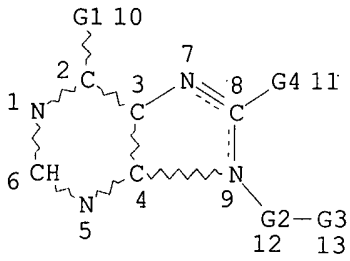
Please note that search-term pricing does apply when conducting SmartSELECT searches.

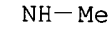
Crossover limits have been increased. See HELP CROSSOVER for details.

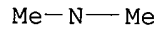
Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

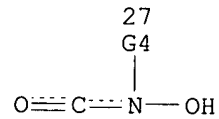
=> d l31 que stat
L1 STR

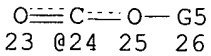
Searched by: Mary Hale 308-4258 CM-1 12D16







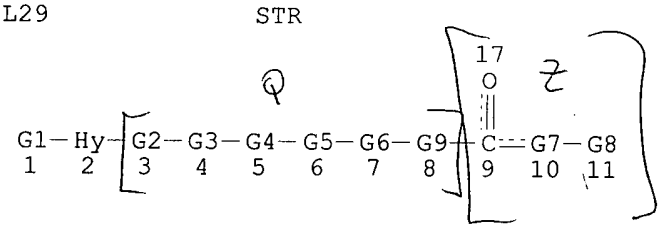


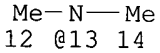


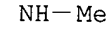
VAR G1=NH2/14/17
REP G2=(1-6) A
VAR G3=20/24
VAR G4=ME/H
VAR G5=H/AK
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

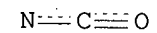
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L29 STR









O @21 N @22

Cy @23

VAR G1=NH2/13/15
VAR G2=18-2 19-4/21/22/23

Searched by: Mary Hale 308-4258 CM-1 12D16

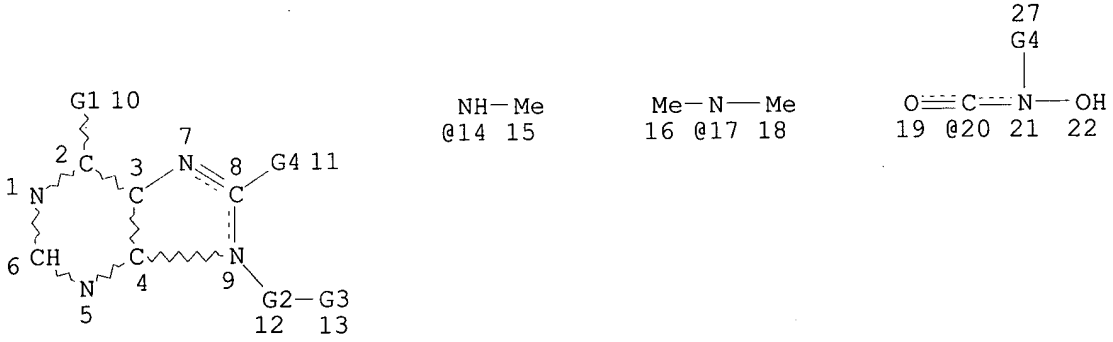
VAR G3=18-3 19-5/21/22/23
VAR G4=18-4 19-6/21/22/23
VAR G5=18-5 19-7/21/22/23
VAR G6=18-6 19-8/21/22/23
VAR G7=O/N
VAR G8=OH/H/AK
VAR G9=18-7 19-9/21/22/23
NODE ATTRIBUTES:
NSPEC IS RC AT 21
NSPEC IS RC AT 22
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY AT 2
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
L31 0 SEA FILE=REGISTRY SSS FUL L1 AND L29

100.0% PROCESSED 36366 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.10

=> d l44 que stat
L1 STR

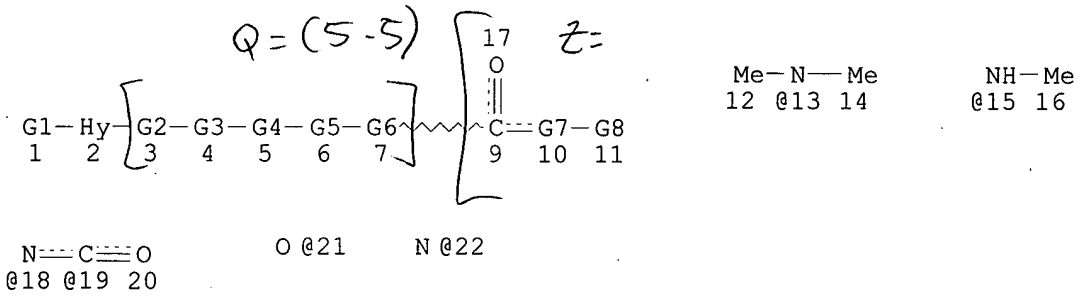


VAR G1=NH2/14/17
REP G2=(1-6) A
VAR G3=20/24
VAR G4=ME/H
VAR G5=H/AK
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L41 STR

Searched by: Mary Hale 308-4258 CM-1 12D16



VAR G1=NH2/13/15
VAR G2=18-2 19-4/21/22/23
VAR G3=18-3 19-5/21/22/23
VAR G4=18-4 19-6/21/22/23
VAR G5=18-5 19-7/21/22/23
VAR G6=18-6 19-9/21/22/23
VAR G7=O/N
VAR G8=OH/H/AK
NODE ATTRIBUTES:
NSPEC IS RC AT 21
NSPEC IS RC AT 22
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY AT 2
DEFAULT ECLEVEL IS LIMITED

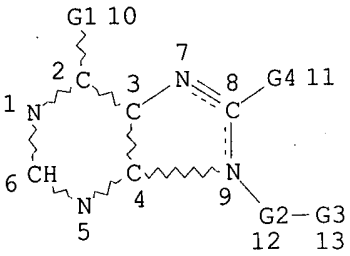
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

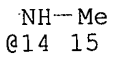
STEREO ATTRIBUTES: NONE
L44 0 SEA FILE=REGISTRY SSS FUL L1 AND L41

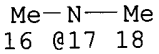
100.0% PROCESSED 36366 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.10

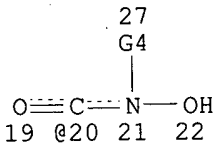
=> d l48 que stat
L1 STR

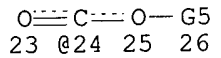
Searched by: Mary Hale 308-4258 CM-1 12D16







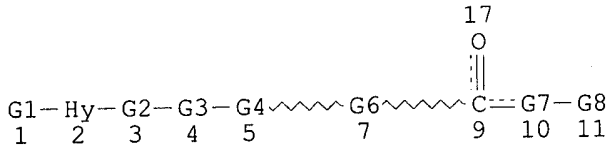


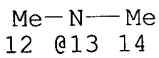


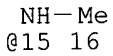
VAR G1=NH2/14/17
REP G2=(1-6) A
VAR G3=20/24
VAR G4=ME/H
VAR G5=H/AK
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

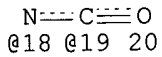
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L45 STR









O @21 N @22

Cy @23

VAR G1=NH2/13/15
VAR G2=18-2 19-4/21/22/23

Searched by: Mary Hale 308-4258 CM-1 12D16

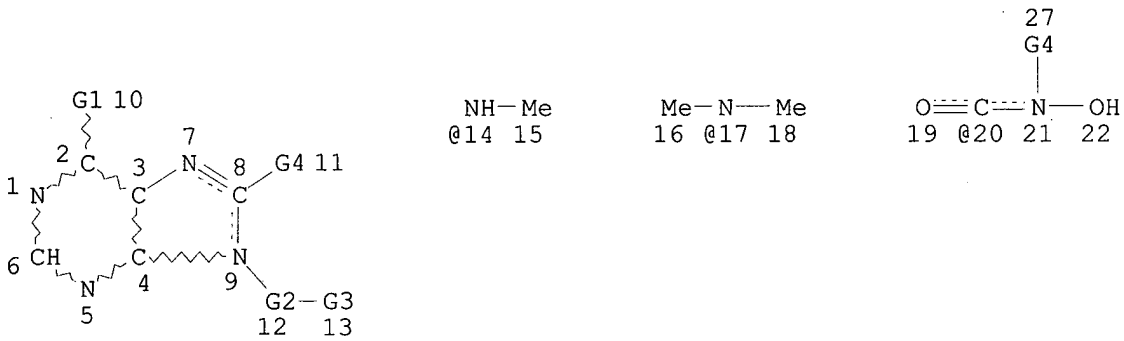
VAR G3=18-3 19-5/21/22/23
VAR G4=18-4 19-7/21/22/23
VAR G6=18-5 19-9/21/22/23
VAR G7=O/N
VAR G8=OH/H/AK
NODE ATTRIBUTES:
NSPEC IS RC AT 21
NSPEC IS RC AT 22
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY AT 2
DEFAULT ECLEVEL IS LIMITED

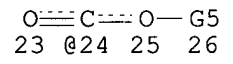
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE
L48 0 SEA FILE=REGISTRY SSS FUL L1 AND L45

100.0% PROCESSED 36366 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.08

=> d l52 que stat
L1 STR



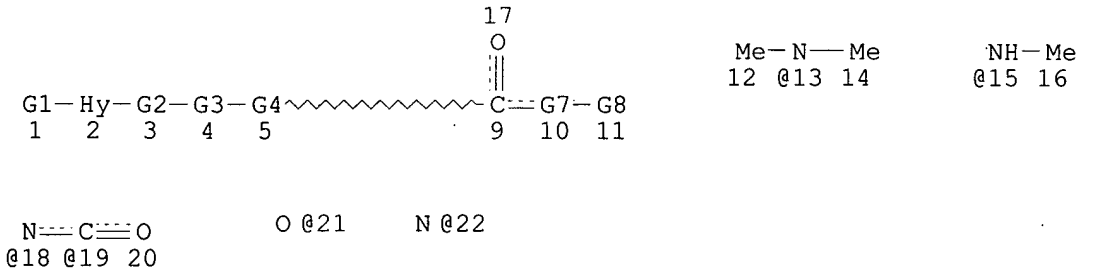


VAR G1=NH2/14/17
REP G2=(1-6) A
VAR G3=20/24
VAR G4=ME/H
VAR G5=H/AK
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L49 STR

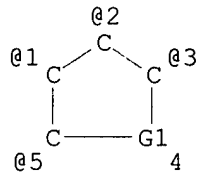
Searched by: Mary Hale 308-4258 CM-1 12D16




```
VAR G1=NH2/13/15
VAR G2=18-2 19-4/21/22/23
VAR G3=18-3 19-5/21/22/23
VAR G4=18-4 19-9/21/22/23
VAR G7=O/N
VAR G8=OH/H/AK
NODE ATTRIBUTES:
NSPEC   IS RC     AT  21
NSPEC   IS RC     AT  22
DEFAULT MLEVEL IS ATOM
GGCAT   IS PCY  AT   2
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  20

STEREO ATTRIBUTES: NONE
L52           0 SEA FILE=REGISTRY SSS FUL L1 AND L49

100.0% PROCESSED  36366 ITERATIONS                        0 ANSWERS
SEARCH TIME: 00.00.08


=> d l62 que stat;d 1-42 ide cbib abs
L2              STR
```

(6)

Searched by: Mary Hale 308-4258 CM-1 12D16



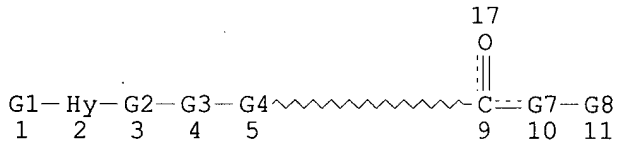
O C Ak
9 @10 11

CH2 O G2
@6 7 8

VAR G1=O/C
VAR G2=H/P/10
VPA 6-3/2/1/5 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC AT 11
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L58 STR



Me N Me
12 @13 14

NH Me
@15 16

N C O
@18 @19 20

O @21

N @22

Cy @23

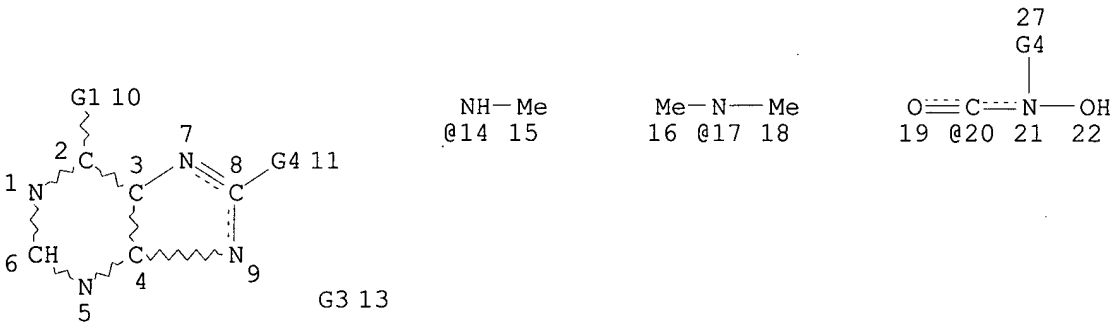
VAR G1=NH2/13/15
VAR G2=18-2 19-4/21/22/23
REP G3=(0-6) A
VAR G4=18-4 19-9/21/22/23
VAR G7=O/N

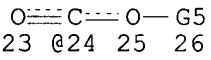
Searched by: Mary Hale 308-4258 CM-1 12D16

VAR G8=OH/H/AK
NODE ATTRIBUTES:
NSPEC IS RC AT 21
NSPEC IS RC AT 22
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY AT 2
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L59 STR





VAR G1=NH2/14/17
VAR G3=20/24
VAR G4=ME/H
VAR G5=H/AK
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE
L62 42 SEA FILE=REGISTRY SSS FUL L59 AND L58 NOT L2

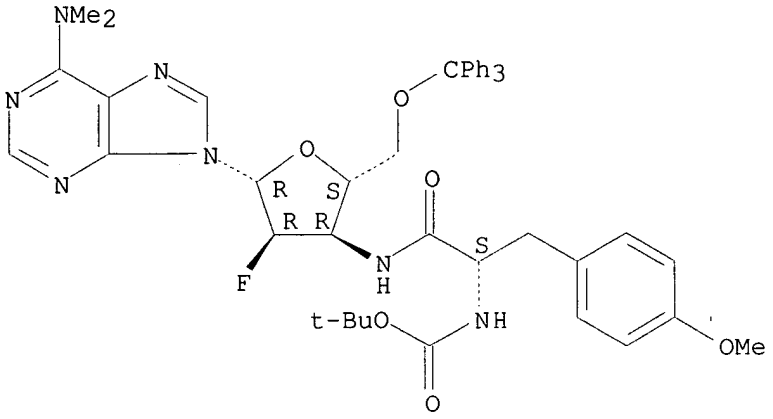
100.0% PROCESSED 36366 ITERATIONS 42 ANSWERS
SEARCH TIME: 00.00.08

L62 ANSWER 1 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 171075-69-7 REGISTRY
CN Adenosine, 2',3'-dideoxy-3'-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-methoxyphenyl)-1-oxopropyl]amino]-2'-fluoro-N,N-dimethyl-5'-O-(triphenylmethyl)-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C46 H50 F N7 O6
SR CA

Searched by: Mary Hale 308-4258 CM-1 12D16

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

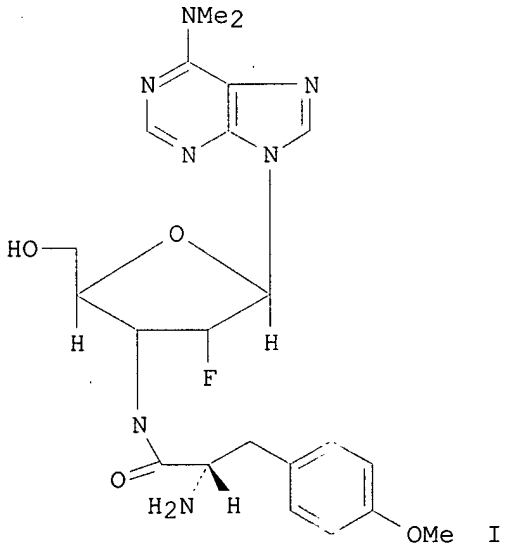


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:9285 Synthesis, antiviral, antibacterial and antitumor cell activities of 2'-deoxy-2'-fluoropuromycin. Maruyama, Tokumi; Utsumi, Kunihiko; Tomioka, Hiroshi; Kasamoto, Masumi; Sato, Yoshiko; Anne, Tozef; de Clercq, Erik (Dep. Pharmaceutical Sciences, Tokushima Bunri Univ., Tokushima, 770, Japan). Chem. Pharm. Bull., 43(6), 955-9 (English) 1995. CODEN: CPBTAL. ISSN: 0009-2363.

GI



I

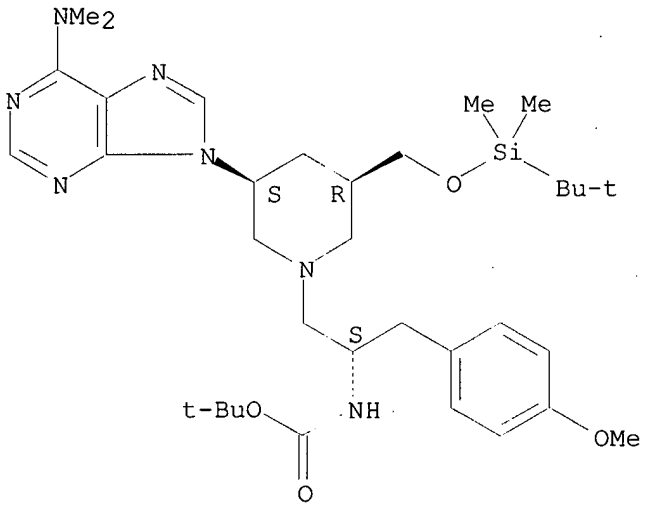
AB A procedure for the synthesis of 2'-deoxy-2'-fluoropuromycin (I) was

Searched by: Mary Hale 308-4258 CM-1 12D16

developed. 2'-Deoxy-2'-fluoropuromycin exhibited no selective antiviral activity against several DNA and RNA viruses. 2'-Deoxy-2'-fluoropuromycin had weak antibacterial activity (min. inhibitory concn. approx. 25-50 .mu.g/mL) and was cytotoxic to several tumor cell lines (L1210, Molt 4, CEM) at a concn. of about 5 .mu.M. This antitumor cell activity may be attributed to inhibition of protein biosynthesis.

L62 ANSWER 2 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 162427-35-2 REGISTRY
CN Carbamic acid, [2-[3-[6-(dimethylamino)-9H-purin-9-yl]-5-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-1-piperidinyl]-1-[(4-methoxyphenyl)methyl]ethyl]-, 1,1-dimethylethyl ester, [3S-[1(R*),3.alpha.,5.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H55 N7 O4 Si
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

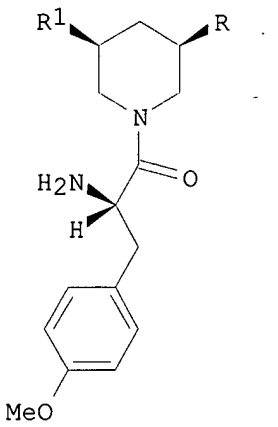


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:240300 Heterocyclic analogs of nucleosides: synthesis and biological evaluation of novel analogs of puromycin. Hultin, Philip G.; Szarek, Walter A. (Dep. Chem., Queen's Univ., Kingston, ON, K7L 3N6, Can.). Can. J. Chem., 72(9), 1978-89 (English) 1994. CODEN: CJCHAG. ISSN: 0008-4042.
GI

Searched by: Mary Hale 308-4258 CM-1 12D16

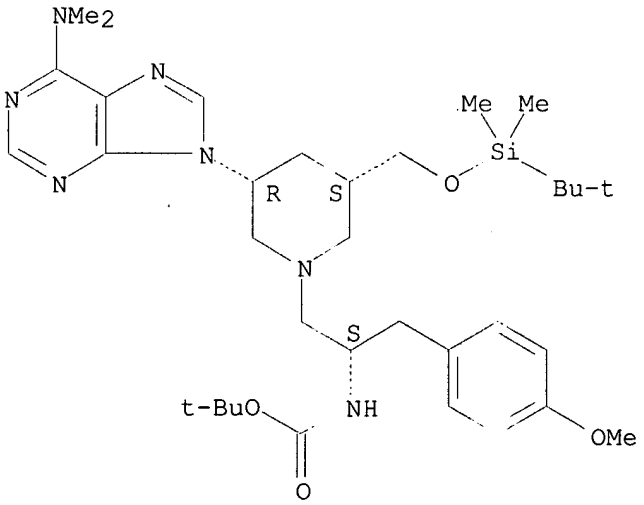


I

AB The diastereomeric 1-(piperidine-3'-yl)uracil compds. and the N6-dimethyl-9-(piperidine-3'-yl)adenine compds. I (R = CH2OH, R1 = uracil, N6-dimethyladenine; R = uracil, N6-dimethyladenine, R1 = CH2OH) have been prepd. as analogs of the naturally occurring aminoacyl nucleoside antibiotic puromycin. The diastereomers were sepd. using HPLC, and the abs. configuration of I were assigned. These puromycin analogs have been tested for anti-HIV and antitumor activity in vitro.

L62 ANSWER 3 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 162315-04-0 REGISTRY
CN Carbamic acid, [2-[3-[6-(dimethylamino)-9H-purin-9-yl]-5-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-1-piperidinyl]-1-[(4-methoxyphenyl)methyl]ethyl]-, 1,1-dimethylethyl ester, [3R-[1(S*),3.alpha.,5.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H55 N7 O4 Si
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



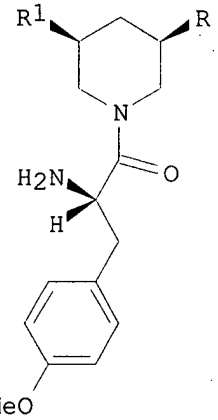
Searched by: Mary Hale 308-4258 CM-1 12D16

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:240300 Heterocyclic analogs of nucleosides: synthesis and biological evaluation of novel analogs of puromycin. Hultin, Philip G.; Szarek, Walter A. (Dep. Chem., Queen's Univ., Kingston, ON, K7L 3N6, Can.). Can. J. Chem., 72(9), 1978-89 (English) 1994. CODEN: CJCHAG. ISSN: 0008-4042.

GI



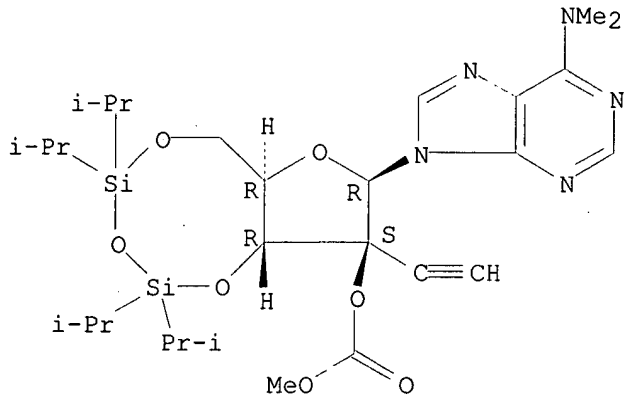
I

AB The diastereomeric 1-(piperidine-3'-yl)uracil compds. and the N6-dimethyl-9-(piperidine-3'-yl)adenine compds. I (R = CH2OH, R1 = uracil, N6-dimethyladenine; R = uracil, N6-dimethyladenine, R1 = CH2OH) have been prepd. as analogs of the naturally occurring aminoacyl nucleoside antibiotic puromycin. The diastereomers were sepd. using HPLC, and the abs. configuration of I were assigned. These puromycin analogs have been tested for anti-HIV and antitumor activity in vitro.

L62 ANSWER 4 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 156569-55-0 REGISTRY
CN 9H-Purin-6-amine, 9-[2-C-ethynyl-2-O-(methoxycarbonyl)-3,5-O-[1,1,3,3-tetrakis(1-methylethyl)-1,3-disiloxanediyl]-.beta.-D-arabinofuranosyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 6H-Furo[3,2-f]-1,3,5,2,4-trioxadisilocin, 9H-purin-6-amine deriv.
FS STEREOSEARCH
MF C28 H45 N5 O7 Si2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

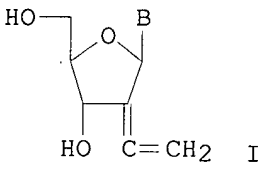
Searched by: Mary Hale 308-4258 CM-1 12D16



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 121:109544 A convenient route to 2'-allenyl nucleosides. Jarvi, Esa T.; McCarthy, James R. (Marion Merrell Dow Res. Inst., Cincinnati, OH, 45215, USA). Nucleosides Nucleotides, 13(1-3), 585-98 (English) 1994. CODEN: NUNUD5. ISSN: 0732-8311.

GI



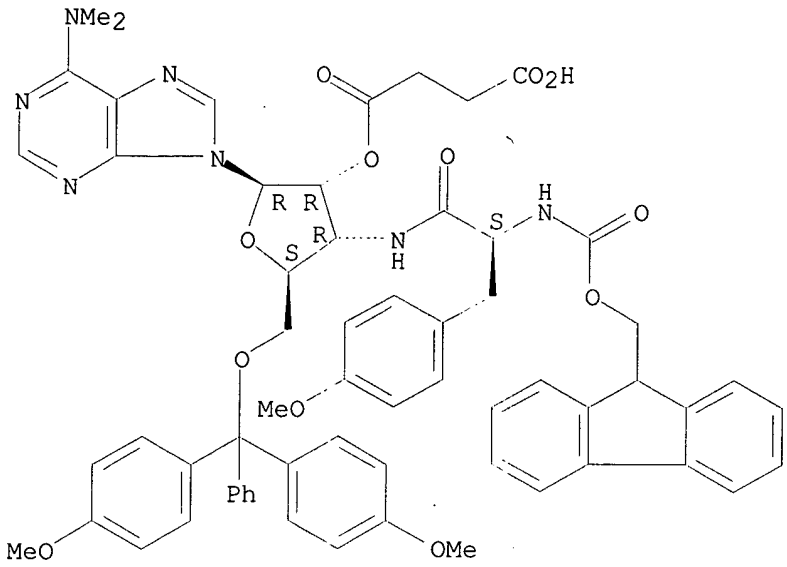
I

AB The first synthesis of allenic nucleosides, e.g. I (B = adenine, cytosine), derived from natural ribonucleosides by a modification of the method developed by Tsuji and co-workers for the synthesis of allenes, is reported. The biol. rationale for the synthesis of these compds. is discussed.

L62 ANSWER 5 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 151967-84-9 REGISTRY
CN Adenosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-deoxy-3'-[[(2S)-2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-(4-methoxyphenyl)-1-oxopropyl]amino]-N,N-dimethyl-, 2'-(hydrogen butanedioate) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Adenosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-deoxy-3'-[[2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-(4-methoxyphenyl)-1-oxopropyl]amino]-N,N-dimethyl-, 2'-(hydrogen butanedioate), (S)-
FS STEREOSEARCH
MF C62 H61 N7 O12
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:267706 Preparation of puromycin-containing nucleic acids by automated solid-phase synthesis, and controlled pore glass supports for it. Sugiyama, Hiroshi; Saito, Akira; Ikeda, Shuji (Tokyo Medical and Dental University, Japan). Jpn. Kokai Tokkyo Koho JP 11071392 A2 19990316 Heisei, 5 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1997-235834 19970901.

AB Title nucleic acids are prepd. by blocking NH2 of puromycin (I) with N-fluorenylmethoxycarbonyl group, blocking 5'-OH with dimethoxytrityl group, binding succinic acid to 3'-OH, reaction of the succinic acid with long-chain alkylamine-controlled pore glass, condensing with nucleotides by the phosphoramidite method, sepg. terminal I-contg. nucleic acids from the supports, deblocking, and purifying. 5'-D(GCAT)-I and 5'-d(CAGGATGGCTTGAAGATGTA)-I were prepd. by the above method.

REFERENCE 2: 129:276214 Facile synthesis of puromycin-tethered oligonucleotides at the 3'-end. Ikeda, Shuji; Saito, Isao; Sugiyama, Hiroshi (Department of Synthetic and Biological Chemistry, Faculty of Engineering, Kyoto University, Kyoto, 606-8501, Japan). Tetrahedron Lett., 39(33), 5975-5978 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB A facile method for the synthesis of puromycin-tethered oligonucleotides at the 3'-end is described. The method utilizes a novel CPG support derived from com. available puromycin. Puromycin-tethered DNA and RNA oligomers were synthesized using a puromycin-tethered CPG support by the usual protocol for automated DNA and RNA synthesis.

REFERENCE 3: 120:77572 Solid phase synthesis of oligonucleotides carrying puromycin at 3'-terminal. Nyilas, Agnes; Agrawal, Sudhir; Zamecnik, Paul (Worcester Found. Exp. Biol., Shrewsbury, MA, 01545, USA). Bioorg. Med. Chem. Lett., 3(6), 1371-4 (English) 1993. CODEN: BMCLE8. ISSN: 0960-894X.

AB For incorporation of puromycin at 3'-end of oligonucleotides or their

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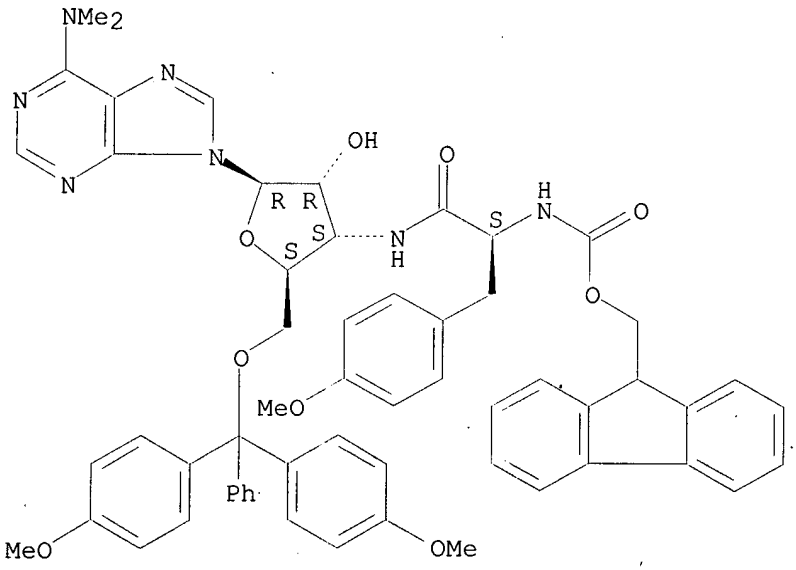
analogs, suitably protected puromycin has been attached to controlled pore glass (CPG).

L62 ANSWER 6 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 151967-83-8 REGISTRY
CN Adenosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-deoxy-3'-[[(2S)-2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-(4-methoxyphenyl)-1-oxopropyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Adenosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-deoxy-3'-[[2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-(4-methoxyphenyl)-1-oxopropyl]amino]-N,N-dimethyl-, (S)-
OTHER NAMES:
CN N-(9-Fluorenylmethoxycarbonyl)-5'-O-dimethoxytritylpuromycin
FS STEREOSEARCH
MF C58 H57 N7 O9
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:267706 Preparation of puromycin-containing nucleic acids by automated solid-phase synthesis, and controlled pore glass supports for it. Sugiyama, Hiroshi; Saito, Akira; Ikeda, Shuji (Tokyo Medical and Dental University, Japan). Jpn. Kokai Tokkyo Koho JP 11071392 A2 19990316 Heisei, 5 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1997-235834 19970901.
AB Title nucleic acids are prepd. by blocking NH2 of puromycin (I) with N-fluorenylmethoxycarbonyl group, blocking 5'-OH with dimethoxytrityl group, binding succinic acid to 3'-OH, reaction of the succinic acid with long-chain alkylamine-controlled pore glass, condensing with nucleotides by the phosphoramidite method, sepg. terminal I-contg. nucleic acids from

the supports, deblocking, and purifying. 5'-D(GCAT)-I and 5'-d(CAGGATGGCTTGAAGATGTA)-I were prepd. by the above method.

REFERENCE 2: 129:276214 Facile synthesis of puromycin-tethered oligonucleotides at the 3'-end. Ikeda, Shuji; Saito, Isao; Sugiyama, Hiroshi (Department of Synthetic and Biological Chemistry, Faculty of Engineering, Kyoto University, Kyoto, 606-8501, Japan). Tetrahedron Lett., 39(33), 5975-5978 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

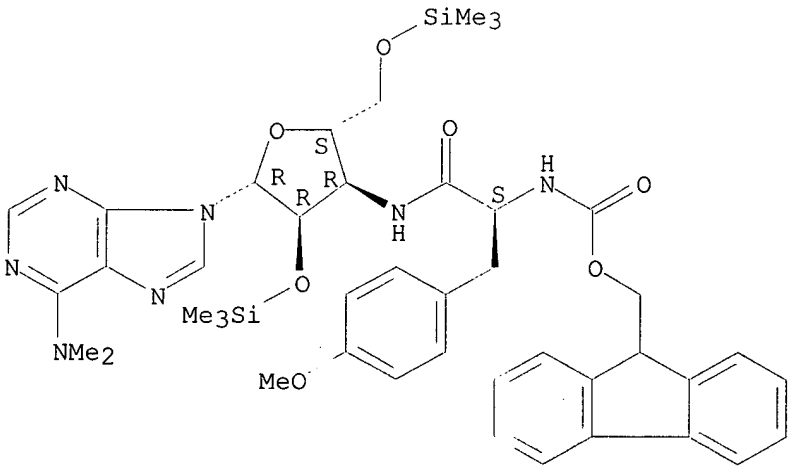
AB A facile method for the synthesis of puromycin-tethered oligonucleotides at the 3'-end is described. The method utilizes a novel CPG support derived from com. available puromycin. Puromycin-tethered DNA and RNA oligomers were synthesized using a puromycin-tethered CPG support by the usual protocol for automated DNA and RNA synthesis.

REFERENCE 3: 120:77572 Solid phase synthesis of oligonucleotides carrying puromycin at 3'-terminal. Nyilas, Agnes; Agrawal, Sudhir; Zamecnik, Paul (Worcester Found. Exp. Biol., Shrewsbury, MA, 01545, USA). Bioorg. Med. Chem. Lett., 3(6), 1371-4 (English) 1993. CODEN: BMCLE8. ISSN: 0960-894X.

AB For incorporation of puromycin at 3'-end of oligonucleotides or their analogs, suitably protected puromycin has been attached to controlled pore glass (CPG).

L62 ANSWER 7 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 151967-81-6 REGISTRY
CN Adenosine, 3'-deoxy-3'-[[2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-(4-methoxyphenyl)-1-oxopropyl]amino]-N,N-dimethyl-2',5'-bis-O-(trimethylsilyl)-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C43 H55 N7 O7 Si2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:77572 Solid phase synthesis of oligonucleotides carrying

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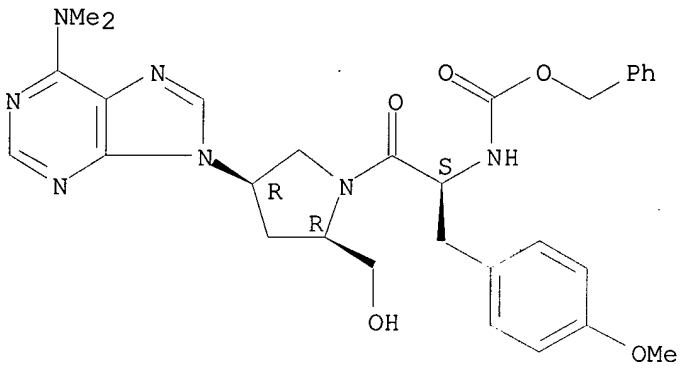
puromycin at 3'-terminal. Nyilas, Agnes; Agrawal, Sudhir; Zamecnik, Paul (Worcester Found. Exp. Biol., Shrewsbury, MA, 01545, USA). Bioorg. Med. Chem. Lett., 3(6), 1371-4 (English) 1993. CODEN: BMCLE8. ISSN: 0960-894X.

AB For incorporation of puromycin at 3'-end of oligonucleotides or their analogs, suitably protected puromycin has been attached to controlled pore glass (CPG).

L62 ANSWER 8 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 135042-35-2 REGISTRY
CN Carbamic acid, [2-[4-[6-(dimethylamino)-9H-purin-9-yl]-2-(hydroxymethyl)-1-pyrrolidinyl]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [2R-[1(S*),2.alpha.,4.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O5
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 115:136560 Synthesis and biological evaluation of 4-purinylpyrrolidine nucleosides. Peterson, Mark L.; Vince, Robert (Coll. Pharm., Univ. Minnesota, Minneapolis, MN, 55455, USA). J. Med. Chem., 34(9), 2787-97 (English) 1991. CODEN: JMCMAR. ISSN: 0022-2623.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis of several novel carbocyclic purine nucleosides which incorporate a nitrogen in place of carbon 3 of the cyclopentyl moiety are described. These analogs are derived from the key stereochem. defined intermediate N-(tert-butoxycarbonyl)-O-[(4-methoxyphenyl)diphenylmethyl]-trans-4-hydroxy-D-prolinol (I), which was accessible in 61.1% overall yield for a five-step sequence starting from cis-4-hydroxy-D-proline. The heterocyclic bases, 6-chloropurine and 2-amino-6-chloropurine, are efficiently introduced onto the pyrrolidine ring via a Mitsunobu-type coupling procedure with Ph3P and di-Et azodicarboxylate. Std.

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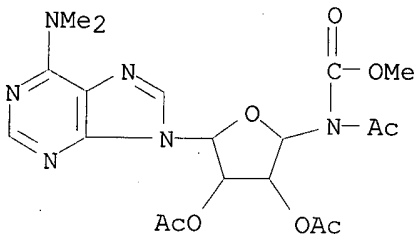
transformations and removal of protecting groups gave the cis-adenine, hypoxanthine, 2,6-diaminopurine, and guanine D-prolinol derivs. II (X = H, Y = NH2, OH; X = NH2, Y = MH2, OH). In addn., a related sequence from trans-4-hydroxy-L-proline provided the enantiomeric L-prolinol guanine deriv. The 6-(dimethylamino)purine analog, was coupled to N-(benzyloxycarbonyl)-p-methoxy-L-phenylalanine to provide, after deprotection, the novel puromycin-like analog III. The analogs II and III were evaluated for antitumor and virucidal activity. These compds. failed to appreciably inhibit the growth of P388 mouse leukemia cells in vitro at concns. up to 100 .mu.g/mL. In addn., they did not exhibit noticeable activity against the HIV or herpes simplex virus type 1 at concns. as high as 100 .mu.M. The adenine analog, I (X = H, Y = NH2) proved to be a substrate for adenosine deaminase and possessed an affinity for the enzyme only 50% less than that of adenosine with a Ki = 85 .mu.M.

L62 ANSWER 9 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 112072-20-5 REGISTRY
CN Adenosine, 5'-N-carboxyacetamido-5'-deoxy-N,N-dimethyl-, methyl ester, diacetate (6CI) (CA INDEX NAME)
MF C19 H24 N6 O8
SR CAOLD
LC STN Files: CAOLD



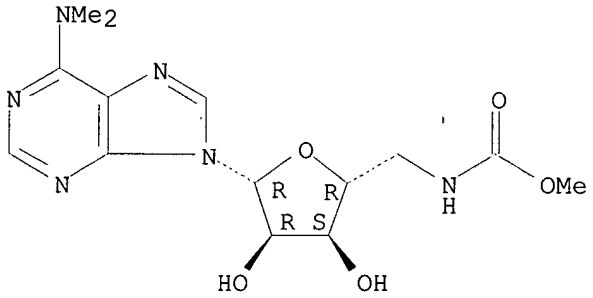
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L62 ANSWER 10 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 109104-86-1 REGISTRY
CN Adenosine, 5'-carboxyamino-5'-deoxy-N,N-dimethyl-, methyl ester (6CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C14 H20 N6 O5
SR CAOLD
LC STN Files: CAOLD

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16

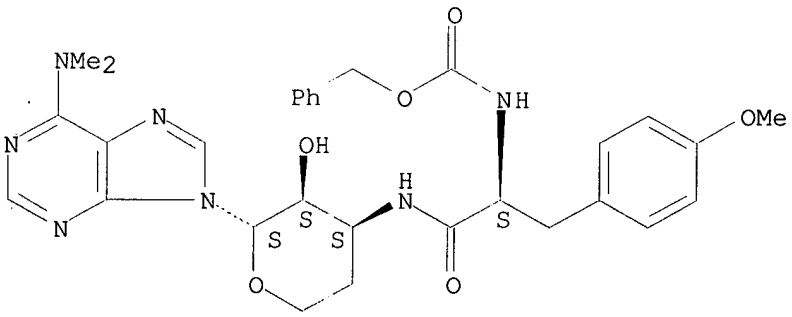


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L62 ANSWER 11 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 87990-07-6 REGISTRY
CN 9H-Purin-6-amine, 9-[3,4-dideoxy-3-[[3-(4-methoxyphenyl)-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-.beta.-L-erythro-pentopyranosyl]-N,N-dimethyl-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O6
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

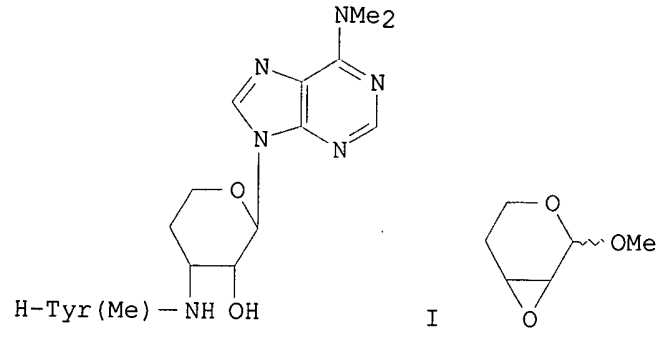


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 100:7088 Route to a pyranic analog of puromycin. Carret, Genevieve; Sarda, Nicole; Abou-Assali, Mounir; Anker, Daniel; Pacheco, Henri (Serv. Chim. Biol., INSA, Villeurbanne, 69621, Fr.). J. Heterocycl. Chem., 20(3), 697-702 (French) 1983. CODEN: JHTCAD. ISSN: 0022-152X.
GI

Searched by: Mary Hale 308-4258 CM-1 12D16



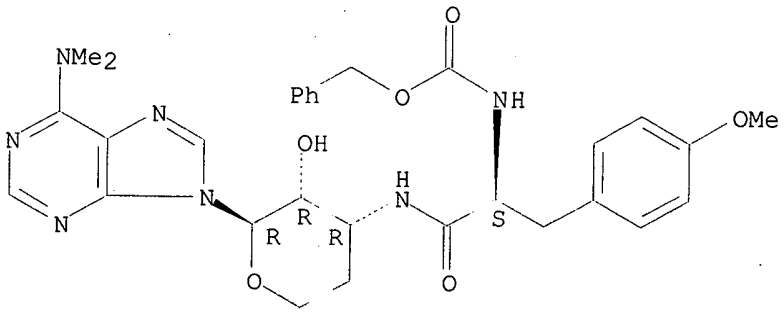
I

II

AB Puromycin pyranic analog I was synthesized by two routes starting from anhydrodeoxypentopyranosides II. In the first method, both amino group and erythro stereochem. were introduced before the introduction of the purine moiety; in the second method, the introduction of the erythro stereochem. and of the 3-nitrogen atom was performed in the same step using an intermediate with a suitable conformation. The two diastereoisomers of I were sepd. and, after assignment of abs. configuration and suitable biol. studies, will permit an evaluation of the role played by the heterocyclic oxygen atom by comparison with previous studies on cyclohexyl puromycin analogs.

L62 ANSWER 12 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 87990-06-5 REGISTRY
CN 9H-Purin-6-amine, 9-[3,4-dideoxy-3-[[3-(4-methoxyphenyl)-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-.beta.-D-erythro-pentopyranosyl]-N,N-dimethyl-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O6
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



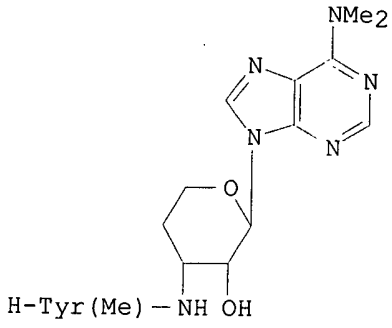
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

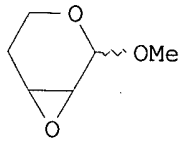
REFERENCE 1: 100:7088 Route to a pyranic analog of puromycin. Carret, Genevieve; Sarda, Nicole; Abou-Assali, Mounir; Anker, Daniel; Pacheco, Henri (Serv. Chim. Biol., INSA, Villeurbanne, 69621, Fr.). J. Heterocycl. Chem., 20(3), 697-702 (French) 1983. CODEN: JHTCAD. ISSN: 0022-152X.

Searched by: Mary Hale 308-4258 CM-1 12D16

GI



I

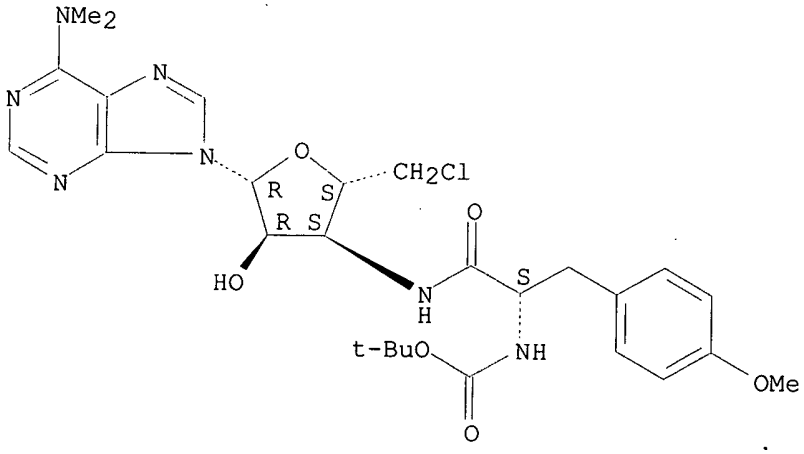


II

AB Puromycin pyranic analog I was synthesized by two routes starting from anhydrodeoxypentopyranosides II. In the first method, both amino group and erythro stereochem. were introduced before the introduction of the purine moiety; in the second method, the introduction of the erythro stereochem. and of the 3-nitrogen atom was performed in the same step using an intermediate with a suitable conformation. The two diastereoisomers of I were sepd. and, after assignment of abs. configuration and suitable biol. studies, will permit an evaluation of the role played by the heterocyclic oxygen atom by comparison with previous studies on cyclohexyl puromycin analogs.

L62 ANSWER 13 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 80361-99-5 REGISTRY
CN Adenosine, 5'-chloro-3',5'-dideoxy-3'-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-methoxyphenyl)-1-oxopropyl]amino]-N,N-dimethyl-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H36 Cl N7 O6
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



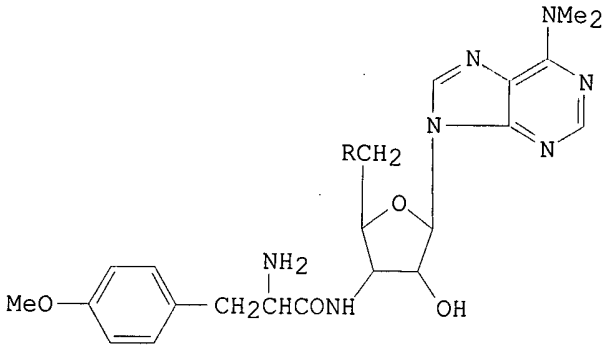
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 12D16

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 96:45905 5'-Chloropuromycin. Inhibition of protein synthesis and antitrypanosomal activity. Vince, Robert; Lee, Heejoo; Narang, A. S.; Shirota, Frances N. (Coll. Pharm., Univ. Minnesota, Minneapolis, MN, 55455, USA). J. Med. Chem., 24(12), 1511-14 (English) 1981. CODEN: JMCMAR. ISSN: 0022-2623.

GI



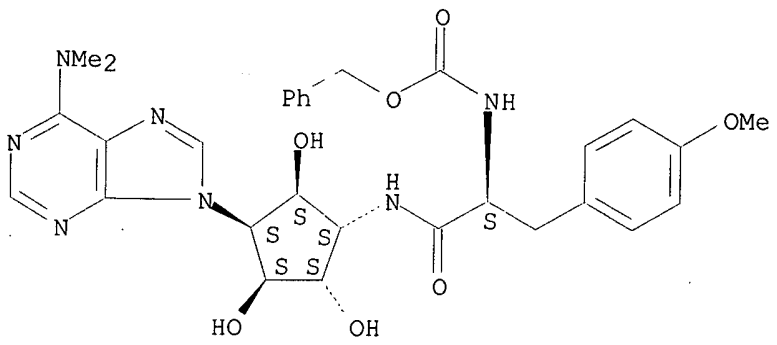
I, R=Cl
II, R=H

AB I [80362-00-1] and II [43157-40-0], puromycin derivs., were synthesized and tested for their ability to inhibit protein formation in vitro and for their antitrypanosomal activity in mice. Both I and II inhibited protein formation by acting as substrates at the peptidyltransferase site of ribosomes, whereas only I exhibited significant antitrypanosomal activity in mice . In rats, the aminonucleosides released by the in vivo hydrolysis of I and II exhibited no nephrotoxicity, whereas the corresponding aminoglycoside of puromycin caused severe nephrotoxic manifestations.

L62 ANSWER 14 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 66574-49-0 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2,4,5-trihydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.beta.,3.beta.,4.beta.,5.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16

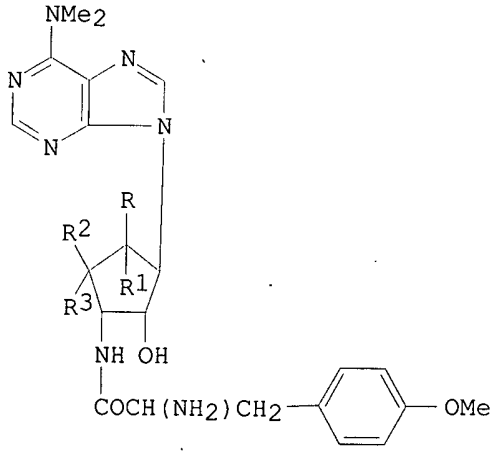


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44054 Nucleoside analogs. 6. A synthesis of carbocyclic puromycin analogs. Suami, Tetsuo; Tadano, Kinichi; Ayabe, Mitsukuni; Emori, Yasufumi (Fac. Eng., Keio Univ., Yokohama, Japan). Bull. Chem. Soc. Jpn., 51(3), 855-61 (English) 1978. CODEN: BCSJA8. ISSN: 0009-2673.

GI



I, R=R3=H, R1=R2=OH
II, R=R3=OH, R1=R2=H

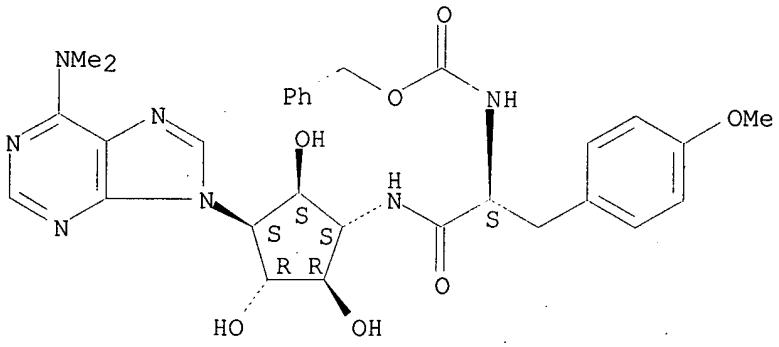
AB Eight carbocyclic puromycin analogs, in which the furanosyl ring of puromycin is replaced with a cyclopentyl system, were prepd. by multi-step sequenceses starting with the reaction of 6-chloro-4-(dimethylamino)-5-nitropyrimidine with 1-amino-3-azido-2,4,5-cyclopentanetriols or 3-acetamido-1-amino-2,4,5-cyclopentanetriols. Their min. degeneration concn. was detd. against HeLa cells in a tissue culture and nucleosides I and II were found to be the most active.

L62 ANSWER 15 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 66574-41-2 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2,4,5-trihydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.beta.,3.beta.,4.alpha.,5.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH

Searched by: Mary Hale 308-4258 CM-1 12D16

MF C30 H35 N7 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44054 Nucleoside analogs. 6. A synthesis of carbocyclic puromycin analogs. Suami, Tetsuo; Tadano, Kinichi; Ayabe, Mitsukuni; Emori, Yasufumi (Fac. Eng., Keio Univ., Yokohama, Japan). Bull. Chem. Soc. Jpn., 51(3), 855-61 (English) 1978. CODEN: BCSJA8. ISSN: 0009-2673.

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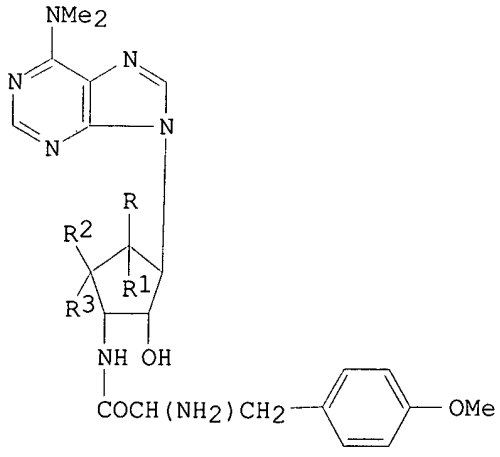


I, R=R3=H, R1=R2=OH
II, R=R3=OH, R1=R2=H

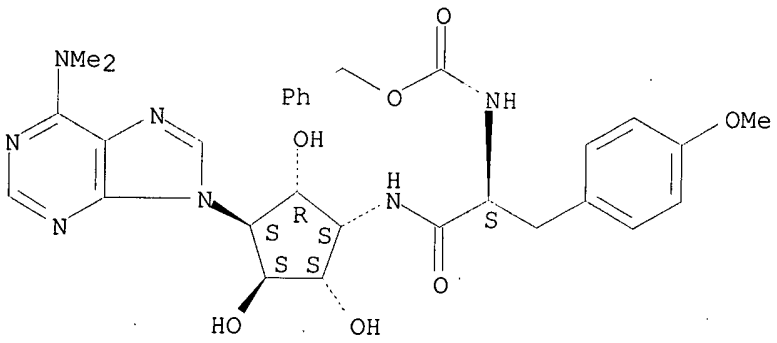
AB Eight carbocyclic puromycin analogs, in which the furanosyl ring of puromycin is replaced with a cyclopentyl system, were prepd. by multi-step sequenceses starting with the reaction of 6-chloro-4-(dimethylamino)-5-nitropyrimidine with 1-amino-3-azido-2,4,5-cyclopentanetriols or 3-acetamido-1-amino-2,4,5-cyclopentanetriols. Their min. degeneration concn. was detd. against HeLa cells in a tissue culture and nucleosides I and II were found to be the most active.

L62 ANSWER 16 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 66574-39-8 REGISTRY

Searched by: Mary Hale 308-4258 CM-1 12D16

CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2,4,5-trihydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.beta.,4.beta.,5.alpha.]]-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.

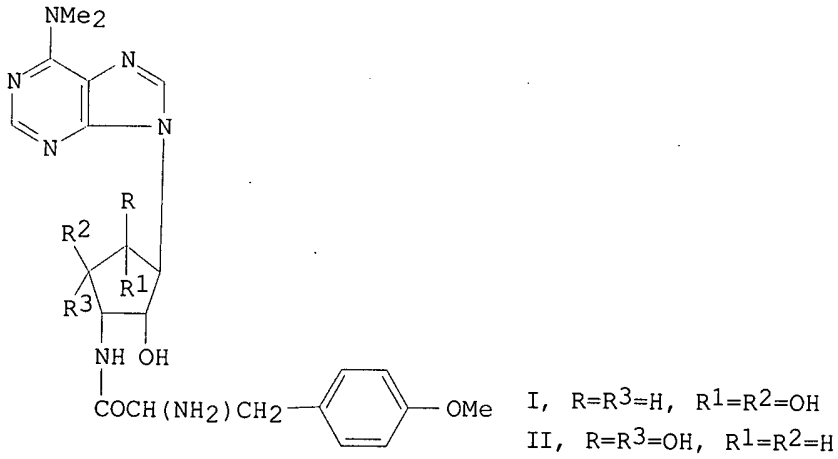


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44054 Nucleoside analogs. 6. A synthesis of carbocyclic puromycin analogs. Suami, Tetsuo; Tadano, Kinichi; Ayabe, Mitsukuni; Emori, Yasufumi (Fac. Eng., Keio Univ., Yokohama, Japan). Bull. Chem. Soc. Jpn., 51(3), 855-61 (English) 1978. CODEN: BCSJA8. ISSN: 0009-2673.

GI



I, R=R3=H, R1=R2=OH
II, R=R3=OH, R1=R2=H

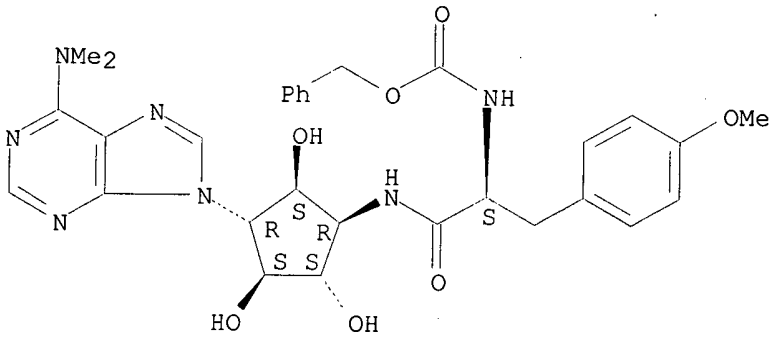
AB Eight carbocyclic puromycin analogs, in which the furanosyl ring of puromycin is replaced with a cyclopentyl system, were prepd. by multi-step sequenceses starting with the reaction of 6-chloro-4-(dimethylamino)-5-nitropyrimidine with 1-amino-3-azido-2,4,5-cyclopentanetriols or 3-acetamido-1-amino-2,4,5-cyclopentanetriols. Their min. degeneration

Searched by: Mary Hale 308-4258 CM-1 12D16

concn. was detd. against HeLa cells in a tissue culture and nucleosides I and II were found to be the most active.

L62 ANSWER 17 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 66574-32-1 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2,4,5-trihydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.alpha.,3.beta.,4.alpha.,5.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44054 Nucleoside analogs. 6. A synthesis of carbocyclic puromycin analogs. Suami, Tetsuo; Tadano, Kinichi; Ayabe, Mitsukuni; Emori, Yasufumi (Fac. Eng., Keio Univ., Yokohama, Japan). Bull. Chem. Soc. Jpn., 51(3), 855-61 (English) 1978. CODEN: BCSJA8. ISSN: 0009-2673.

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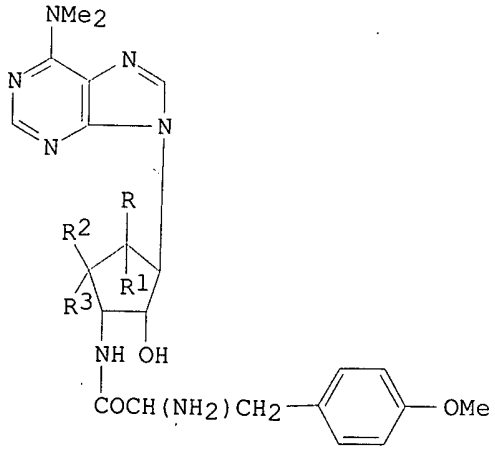


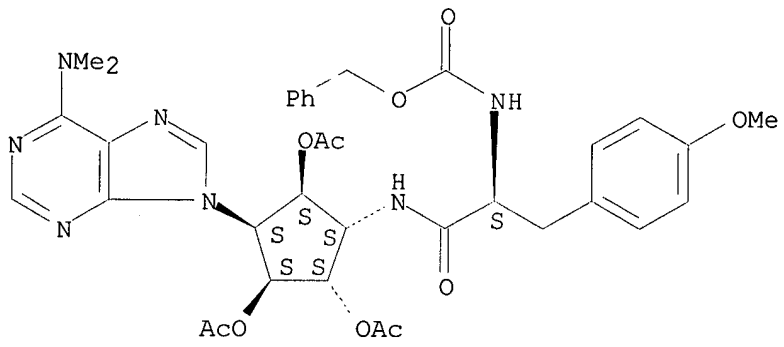
I, R=R3=H, R1=R2=OH
II, R=R3=OH, R1=R2=H

Searched by: Mary Hale 308-4258 CM-1 12D16

AB Eight carbocyclic puromycin analogs, in which the furanosyl ring of puromycin is replaced with a cyclopentyl system, were prepd. by multi-step sequenceses starting with the reaction of 6-chloro-4-(dimethylamino)-5-nitropyrimidine with 1-amino-3-azido-2,4,5-cyclopentanetriols or 3-acetamido-1-amino-2,4,5-cyclopentanetriols. Their min. degeneration concn. was detd. against HeLa cells in a tissue culture and nucleosides I, and II were found to be the most active.

L62 ANSWER 18 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 66530-30-1 REGISTRY
CN Carbamic acid, [1-[(4-methoxyphenyl)methyl]-2-oxo-2-[[2,3,5-tris(acetyloxy)-4-[6-(dimethylamino)-9H-purin-9-yl]cyclopentyl]amino]ethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.beta.,4.beta.,5.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C36 H41 N7 O10
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.

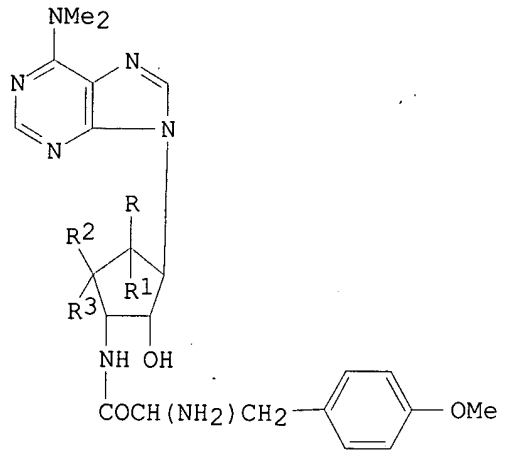


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44054 Nucleoside analogs. 6. A synthesis of carbocyclic puromycin analogs. Suami, Tetsuo; Tadano, Kinichi; Ayabe, Mitsukuni; Emori, Yasufumi (Fac. Eng., Keio Univ., Yokohama, Japan). Bull. Chem. Soc. Jpn., 51(3), 855-61 (English) 1978. CODEN: BCSJA8. ISSN: 0009-2673.
GI

Searched by: Mary Hale 308-4258 CM-1 12D16

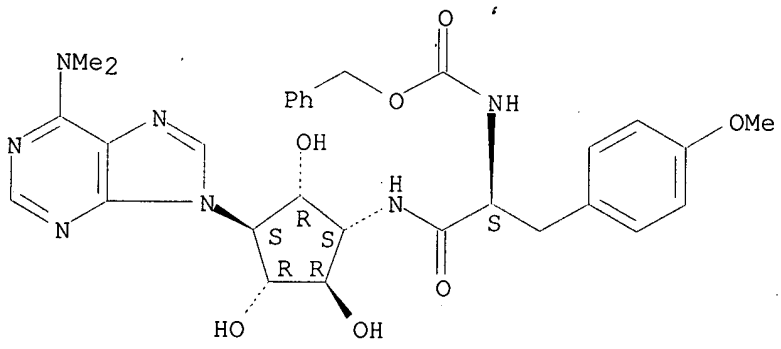


I, R=R3=H, R1=R2=OH
II, R=R3=OH, R1=R2=H

AB Eight carbocyclic puromycin analogs, in which the furanosyl ring of puromycin is replaced with a cyclopentyl system, were prepd. by multi-step sequenceses starting with the reaction of 6-chloro-4-(dimethylamino)-5-nitropyrimidine with 1-amino-3-azido-2,4,5-cyclopentanetriols or 3-acetamido-1-amino-2,4,5-cyclopentanetriols. Their min. degeneration concn. was detd. against HeLa cells in a tissue culture and nucleosides I and II were found to be the most active.

L62 ANSWER 19 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 66530-25-4 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2,4,5-trihydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.beta.,4.alpha.,5.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

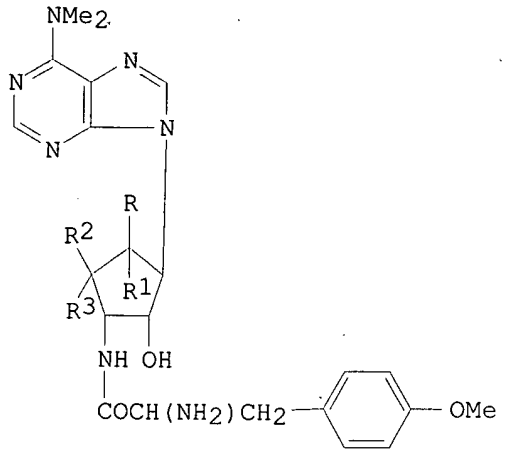
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44054 Nucleoside analogs. 6. A synthesis of carbocyclic

Searched by: Mary Hale 308-4258 CM-1 12D16

puromycin analogs. Suami, Tetsuo; Tadano, Kinichi; Ayabe, Mitsukuni; Emori, Yasufumi (Fac. Eng., Keio Univ., Yokohama, Japan). Bull. Chem. Soc. Jpn., 51(3), 855-61 (English) 1978. CODEN: BCSJA8. ISSN: 0009-2673.

GI

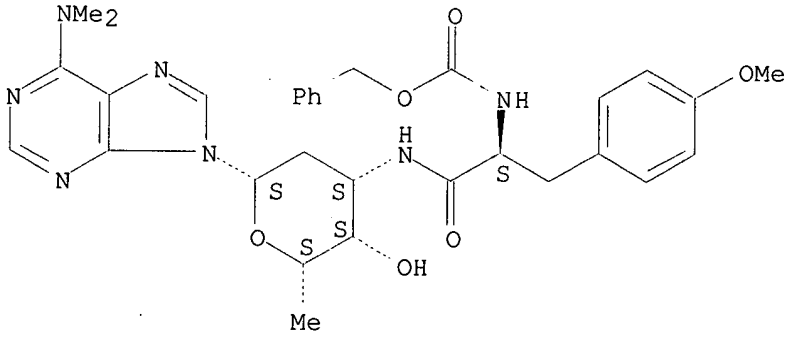


I, R=R3=H, R1=R2=OH
II, R=R3=OH, R1=R2=H

AB Eight carbocyclic puromycin analogs, in which the furanosyl ring of puromycin is replaced with a cyclopentyl system, were prepd. by multi-step sequenceses starting with the reaction of 6-chloro-4-(dimethylamino)-5-nitropyrimidine with 1-amino-3-azido-2,4,5-cyclopentanetriols or 3-acetamido-1-amino-2,4,5-cyclopentanetriols. Their min. degeneration concn. was detd. against HeLa cells in a tissue culture and nucleosides I and II were found to be the most active.

L62 ANSWER 20 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 63622-03-7 REGISTRY
CN 9H-Purin-6-amine, N,N-dimethyl-9-[2,3,6-trideoxy-3-[[3-(4-methoxyphenyl)-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-.beta.-L-lyxo-hexopyranosyl]-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H37 N7 O6
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



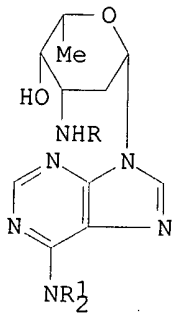
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 12D16

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:85194 Synthesis of some purine and pyrimidine nucleosides of 3-amino-2,3,6-trideoxy-L-lyxo-hexopyranose (daunosamine). Lazzari, Ettore; Vigevani, Aristide; Arcamone, Federico (Res. Lab., Farmitalia, Milan, Italy). Carbohydr. Res., 56(1), 35-42 (English) 1977. CODEN: CRBRAT.

GI



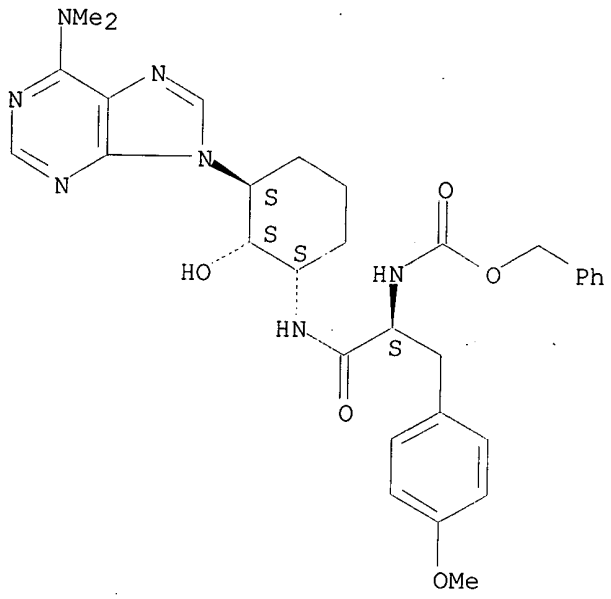
I

AB The daunosaminyl analog of puromycin and the nucleoside derivs. of 6-dimethylaminopurine, thymine, and cytosine were prepd. by melting the protected daunosamine with the protected base in vacuo. Thus, I (R = R1 = H) was prepd. by condensation of N,O-ditrifluoroacetyl-.alpha.-daunosaminyl chloride with either N6-benzoyl-9-chloromercuriadenine or N6-benzoyladenine. Coupling of I (R = H, R1 = Me) with PhCH2O2C-Tyr(OMe)-OH followed by hydrogenolysis gave the daunosaminyl analog I (R = 4-MeOC6H4CH2CH(NH2)CO, R1 = Me) of puromycin.

L62 ANSWER 21 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 62989-86-0 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclohexyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H37 N7 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16

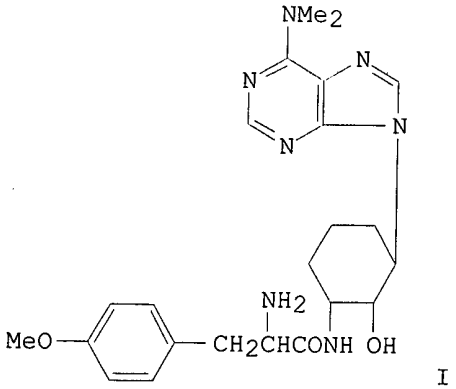


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:63341 Synthesis of cyclohexyl carbocyclic puromycin and its inhibition of protein synthesis. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 20(7), 930-4 (English) 1977. CODEN: JMCMAR.

GI



I

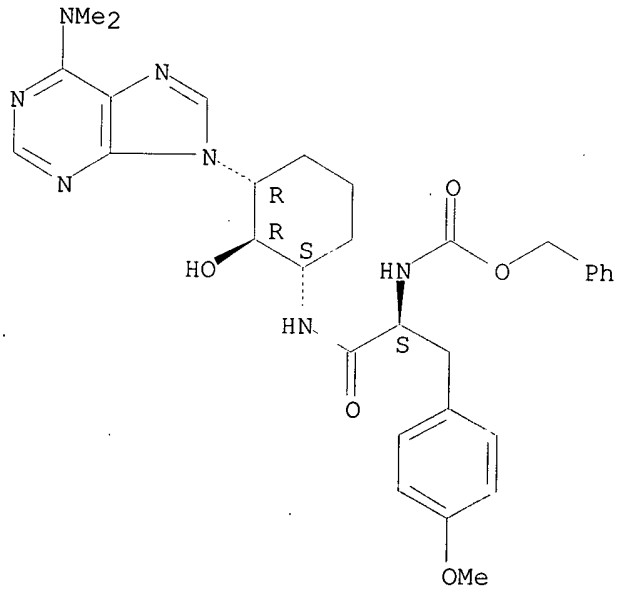
AB Four title compds., 6-dimethylamino-9-[(R)-[2(R)-hydroxy-3(R)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine (I) [62854-09-5], 6-dimethylamino-9-[(S)-[2(S)-hydroxy-3(S)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-90-9], 6-dimethylamino-9-[(R)-[2(R)-hydroxy-3(S)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-87-4], and 6-dimethylamino-9-[(S)-[2(S)-hydroxy-3(R)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-91-0], were prepd. Of the above compds. and 2 trans-cyclopentyl carbocyclic puromycin

Searched by: Mary Hale 308-4258 CM-1 12D16

analogs, all but I were inactive at 10-3 M as inhibitors of poly(U,C)-directed L-[14C]poly(phenylalanine) formation in an Escherichia coli cell-free ribosome system. I had a 45-fold lower activity than puromycin [53-79-2] in the same system in comparisons of 50% inhibition concns. Apparently, max. activity of puromycin analogs is obtained when the purine moiety, amino acid, and hydroxyl group are oriented about a 5-membered ring. The amino acid and hydroxyl group must be in a cis orientation, and the abs. stereochem. of the parent antibiotic must be conserved.

L62 ANSWER 22 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 62960-65-0 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclohexyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.beta.,3.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H37 N7 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

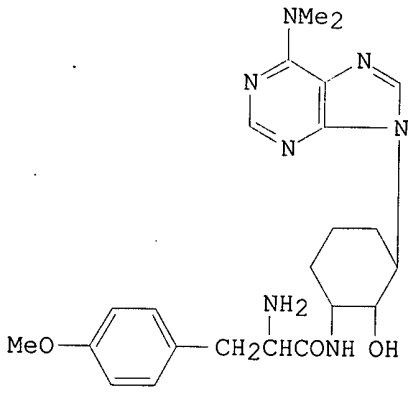


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:63341 Synthesis of cyclohexyl carbocyclic puromycin and its inhibition of protein synthesis. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 20(7), 930-4 (English) 1977. CODEN: JMCMAR.
GI

Searched by: Mary Hale 308-4258 CM-1 12D16



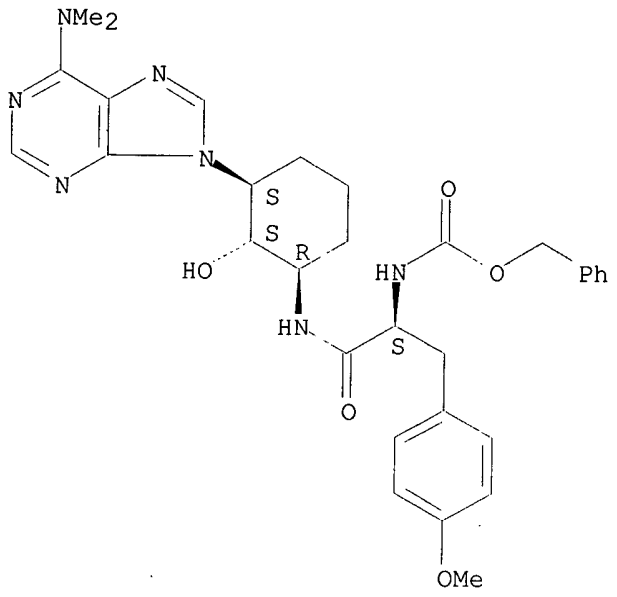
I

AB Four title compds., 6-dimethylamino-9-[(R)-[2(R)-hydroxy-3(R)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine (I) [62854-09-5], 6-dimethylamino-9-[(S)-[2(S)-hydroxy-3(S)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-90-9], 6-dimethylamino-9-[(R)-[2(R)-hydroxy-3(S)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-87-4], and 6-dimethylamino-9-[(S)-[2(S)-hydroxy-3(R)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-91-0], were prepd. Of the above compds. and 2 trans-cyclopentyl carbocyclic puromycin analogs, all but I were inactive at 10-3 M as inhibitors of poly(U,C)-directed L-[14C]poly(phenylalanine) formation in an Escherichia coli cell-free ribosome system. I had a 45-fold lower activity than puromycin [53-79-2] in the same system in comparisons of 50% inhibition concns. Apparently, max. activity of puromycin analogs is obtained when the purine moiety, amino acid, and hydroxyl group are oriented about a 5-membered ring. The amino acid and hydroxyl group must be in a cis orientation, and the abs. stereochem. of the parent antibiotic must be conserved.

L62 ANSWER 23 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 62854-19-7 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclohexyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.beta.,3.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H37 N7 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16

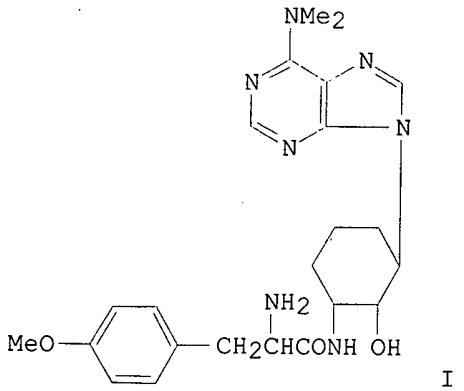


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:63341 Synthesis of cyclohexyl carbocyclic puromycin and its inhibition of protein synthesis. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 20(7), 930-4 (English) 1977. CODEN: JMCMAR.

GI



I

AB Four title compds., 6-dimethylamino-9-[(R)-[2(R)-hydroxy-3(R)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine (I) [62854-09-5], 6-dimethylamino-9-[(S)-[2(S)-hydroxy-3(S)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-90-9], 6-dimethylamino-9-[(R)-[2(R)-hydroxy-3(S)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-87-4], and 6-dimethylamino-9-[(S)-[2(S)-hydroxy-3(R)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-91-0], were prepd. Of the above compds. and 2 trans-cyclopentyl carbocyclic puromycin

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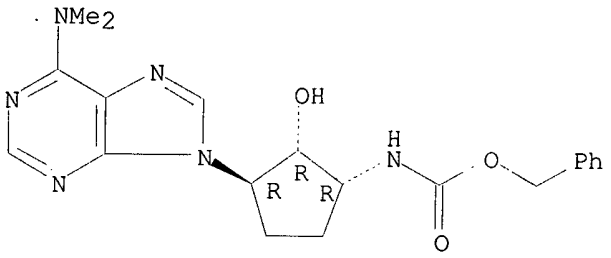
analogs, all but I were inactive at 10-3 M as inhibitors of poly(U,C)-directed L-[14C]poly(phenylalanine) formation in an Escherichia coli cell-free ribosome system. I had a 45-fold lower activity than puromycin [53-79-2] in the same system in comparisons of 50% inhibition concns. Apparently, max. activity of puromycin analogs is obtained when the purine moiety, amino acid, and hydroxyl group are oriented about a 5-membered ring. The amino acid and hydroxyl group must be in a cis orientation, and the abs. stereochem. of the parent antibiotic must be conserved.

L62 ANSWER 24 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 54700-35-5 REGISTRY
CN Carbamic acid, [3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]-, phenylmethyl ester, (1.alpha.,2.alpha.,3.beta.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Carbamic acid, [3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]-, phenylmethyl ester, (1.alpha.,2.alpha.,3.beta.)-(.+-.)-
FS STEREOSEARCH
MF C20 H24 N6 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

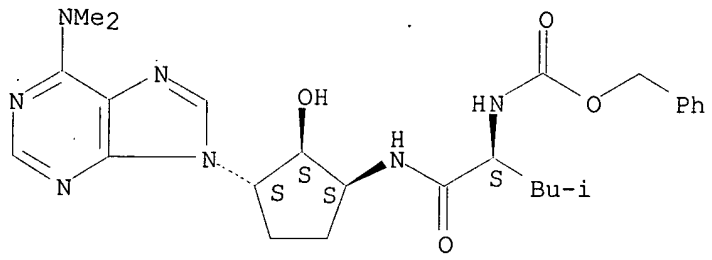
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 82:58074 (+-)-9-.beta.-(3-.alpha.-Amino-2.alpha.-hydroxy cyclopentyl)-6-substituted-purines and derivatives. Vince, Robert (University of Minnesota). U.S. US 3825541 19740723, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1972-220890 19720126.
GI For diagram(s), see printed CA Issue.
AB Pyromycin analogs (I and II) possessing bactericidal, antiprotozoan and anticancer activity were prepd. via coupling (.+-.)-9-[.beta.-(3.alpha.-amino-2.alpha.-hydroxy)cyclopentyl]-6-(dimethylamino)purine with N-benzyloxycarbonyl-p-methoxyphenyl-L-alanine. One isomer, assumed to be I, exhibited bactericidal activity equiv. to puromycin, whereas II was completely inactive.

L62 ANSWER 25 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 52691-29-9 REGISTRY
CN Carbamic acid, [1-[[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H35 N7 O4
LC STN Files: CA, CAPLUS

Searched by: Mary Hale 308-4258 CM-1 12D16

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

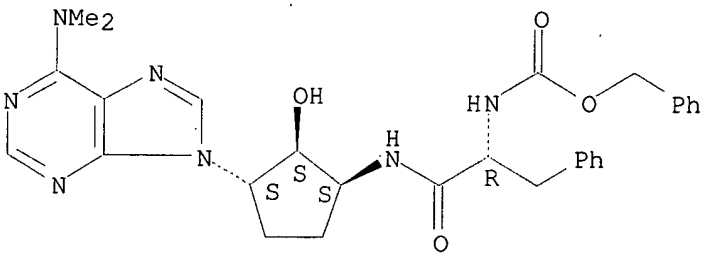
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:115149 Puromycin analogs. Ribosomal binding with diastereomeric carbocyclic puromycin analogs. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 17(6), 578-83 (English) 1974. CODEN: JMCMAR.

AB Of 7 title compds. prepd. and found active in the inhibition of poly-UC-directed polyphenylalanine formation in an Escherichia coli cell-free system, 6-(dimethylamino)-9-[(R)-[(2R)-hydroxy-(3R)-(L-phenylalanylamino)]cyclopentyl]purine (I) [52661-26-4] gave 98.6% inhibition at 10-4M. I was prepd. from 3-acetamidocyclopentene [52661-16-2] by epoxidn., opening of the epoxide with NaN3 [26628-22-8], followed by redn. to the azido alc., resoln. via tartrate formation, introduction of the purine moiety, and coupling with the amino acid. The relation of structure of the various aminoacyl analogs to activity was discussed.

L62 ANSWER 26 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 52691-28-8 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, [1S-[1.alpha.(S*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H33 N7 O4
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 12D16

REFERENCE 1: 81:115149 Puromycin analogs. Ribosomal binding with diastereomeric carbocyclic puromycin analogs. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 17(6), 578-83 (English) 1974. CODEN: JMCMAR.

AB Of 7 title compds. prepd. and found active in the inhibition of poly-UC-directed polyphenylalanine formation in an Escherichia coli cell-free system, 6-(dimethylamino)-9-[(R)-[(2R)-hydroxy-(3R)-(L-phenylalanylamino)]cyclopentyl]purine (I) [52661-26-4] gave 98.6% inhibition at 10-4M. I was prepd. from 3-acetamidocyclopentene [52661-16-2] by epoxidn., opening of the epoxide with NaN3 [26628-22-8], followed by redn. to the azido alc., resoln. via tartrate formation, introduction of the purine moiety, and coupling with the amino acid. The relation of structure of the various aminoacyl analogs to activity was discussed.

L62 ANSWER 27 OF 42 REGISTRY COPYRIGHT 2002 ACS

RN 52691-27-7 REGISTRY

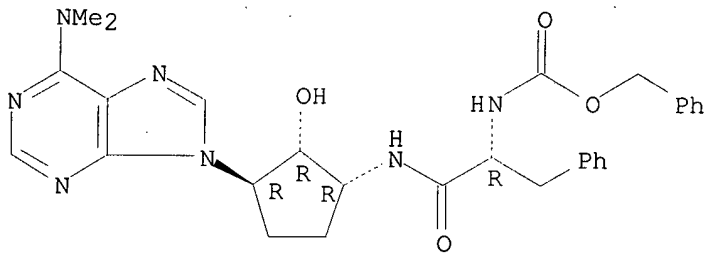
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, [1R-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H33 N7 O4

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:115149 Puromycin analogs. Ribosomal binding with diastereomeric carbocyclic puromycin analogs. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 17(6), 578-83 (English) 1974. CODEN: JMCMAR.

AB Of 7 title compds. prepd. and found active in the inhibition of poly-UC-directed polyphenylalanine formation in an Escherichia coli cell-free system, 6-(dimethylamino)-9-[(R)-[(2R)-hydroxy-(3R)-(L-phenylalanylamino)]cyclopentyl]purine (I) [52661-26-4] gave 98.6% inhibition at 10-4M. I was prepd. from 3-acetamidocyclopentene [52661-16-2] by epoxidn., opening of the epoxide with NaN3 [26628-22-8], followed by redn. to the azido alc., resoln. via tartrate formation, introduction of the purine moiety, and coupling with the amino acid. The relation of structure of the various aminoacyl analogs to activity was discussed.

L62 ANSWER 28 OF 42 REGISTRY COPYRIGHT 2002 ACS

RN 52691-26-6 REGISTRY

CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl

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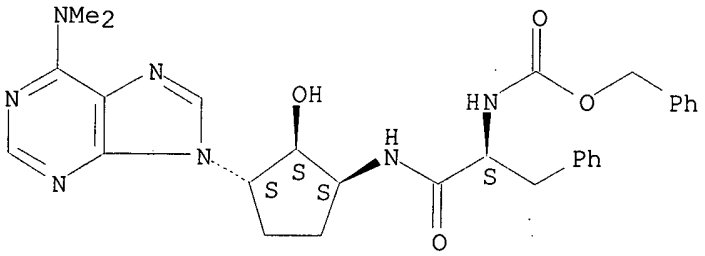
ester, [1S-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H33 N7 O4
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



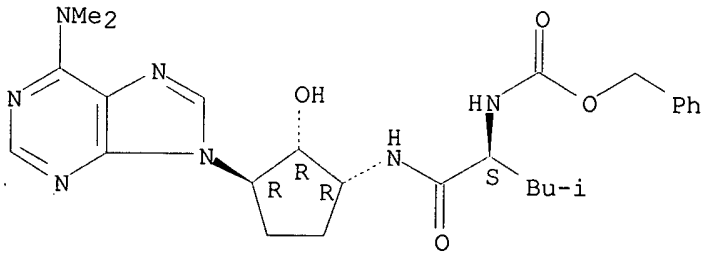
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:115149 Puromycin analogs. Ribosomal binding with diastereomeric carbocyclic puromycin analogs. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 17(6), 578-83 (English) 1974. CODEN: JMCMAR.
AB Of 7 title compds. prepd. and found active in the inhibition of poly-UC-directed polyphenylalanine formation in an Escherichia coli cell-free system, 6-(dimethylamino)-9-[(R)-[(2R)-hydroxy-(3R)-(L-phenylalanylamino)]cyclopentyl]purine (I) [52661-26-4] gave 98.6% inhibition at 10-4M. I was prepd. from 3-acetamidocyclopentene [52661-16-2] by epoxidn., opening of the epoxide with NaN3 [26628-22-8], followed by redn. to the azido alc., resoln. via tartrate formation, introduction of the purine moiety, and coupling with the amino acid. The relation of structure of the various aminoacyl analogs to activity was discussed.

L62 ANSWER 29 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 52661-25-3 REGISTRY
CN Carbamic acid, [1-[[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H35 N7 O4
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



Searched by: Mary Hale 308-4258 CM-1 12D16

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

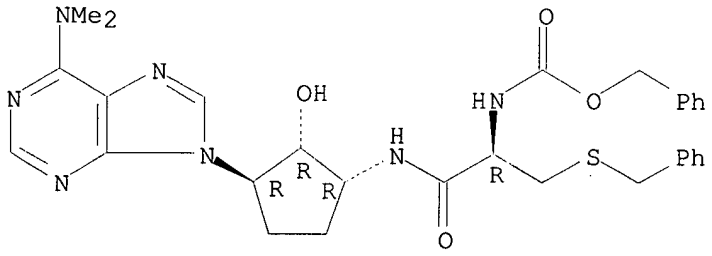
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:115149 Puromycin analogs. Ribosomal binding with diastereomeric carbocyclic puromycin analogs. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 17(6), 578-83 (English) 1974. CODEN: JMCMAR.

AB Of 7 title compds. prepd. and found active in the inhibition of poly-UC-directed polyphenylalanine formation in an Escherichia coli cell-free system, 6-(dimethylamino)-9-[(R)-[(2R)-hydroxy-(3R)-(L-phenylalanylamino)]cyclopentyl]purine (I) [52661-26-4] gave 98.6% inhibition at 10-4M. I was prepd. from 3-acetamidocyclopentene [52661-16-2] by epoxidn., opening of the epoxide with NaN3 [26628-22-8], followed by redn. to the azido alc., resoln. via tartrate formation, introduction of the purine moiety, and coupling with the amino acid. The relation of structure of the various aminoacyl analogs to activity was discussed.

L62 ANSWER 30 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 52661-24-2 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-[[(phenylmethyl)thio]methyl]ethyl]-, phenylmethyl ester, [1R-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O4 S
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:115149 Puromycin analogs. Ribosomal binding with diastereomeric carbocyclic puromycin analogs. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 17(6), 578-83 (English) 1974. CODEN: JMCMAR.

AB Of 7 title compds. prepd. and found active in the inhibition of poly-UC-directed polyphenylalanine formation in an Escherichia coli cell-free system, 6-(dimethylamino)-9-[(R)-[(2R)-hydroxy-(3R)-(L-phenylalanylamino)]cyclopentyl]purine (I) [52661-26-4] gave 98.6% inhibition at 10-4M. I was prepd. from 3-acetamidocyclopentene [52661-16-2] by epoxidn., opening of the epoxide with NaN3 [26628-22-8], followed by redn. to the azido alc., resoln. via tartrate formation, introduction of the purine moiety, and coupling with the amino acid. The relation of structure of the various aminoacyl analogs to activity was

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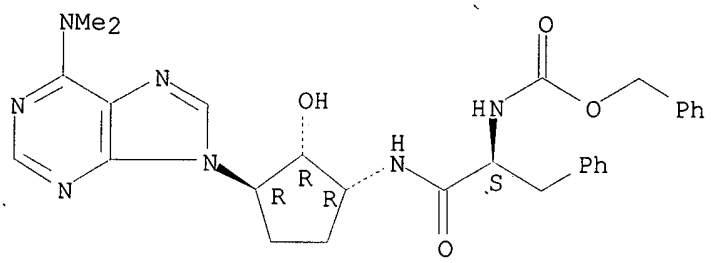
discussed.

L62 ANSWER 31 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 52661-23-1 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H33 N7 O4
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

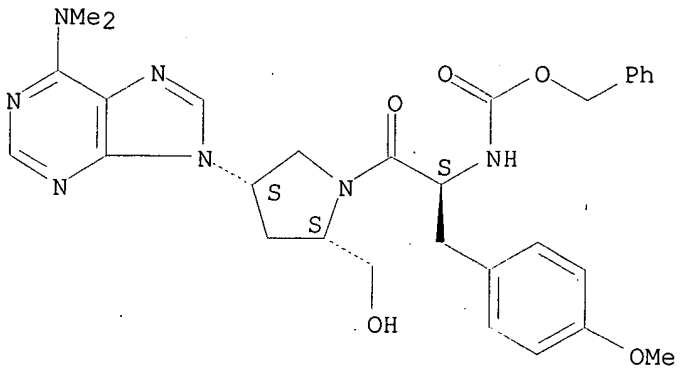
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:115149 Puromycin analogs. Ribosomal binding with diastereomeric carbocyclic puromycin analogs. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 17(6), 578-83 (English) 1974. CODEN: JMCMAR.
AB Of 7 title compds. prepd. and found active in the inhibition of poly-UC-directed polyphenylalanine formation in an Escherichia coli cell-free system, 6-(dimethylamino)-9-[(R)-[(2R)-hydroxy-(3R)-(L-phenylalanylamino)]cyclopentyl]purine (I) [52661-26-4] gave 98.6% inhibition at 10-4M. I was prepd. from 3-acetamidocyclopentene [52661-16-2] by epoxidn., opening of the epoxide with NaN3 [26628-22-8], followed by redn. to the azido alc., resoln. via tartrate formation, introduction of the purine moiety, and coupling with the amino acid. The relation of structure of the various aminoacyl analogs to activity was discussed.

L62 ANSWER 32 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 51846-78-7 REGISTRY
CN Carbamic acid, [2-[4-[6-(dimethylamino)-9H-purin-9-yl]-2-(hydroxymethyl)-1-pyrrolidinyl]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [2S-[1(R*),2.alpha.,4.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 80:108480 Unconventional nucleotide analogs. XI. Synthesis of a nonsaccharidal analog of puromycin. Kaspersen, Frans M.; Bieraugel, Hans; Pandit, Upendra K. (Org. Chem. Lab., Univ. Amsterdam, Amsterdam, Neth.). Heterocycles, 2(1), 15-19 (English) 1974. CODEN: HTCYAM.

GI For diagram(s), see printed CA Issue.

AB The title puromycin analog (I), of interest because of analogy to nucleo-peptide models, is prepd. Thus, (-)-4-hydroxy-L-proline was converted to II which on treatment with 5-amino-4,6-dichloropyrimidine followed by ring closure [(EtO)3CH] gave III (R = Cl, R1 = tosyl). Reaction of this with Me2NH and detosylation gave III (R = NMe2, R1 = H). Coupling of this with Cbz N-protected 4-MeOC6H4CH2CH(NH2)-CO2H gave, after removal of the Cbz group, I.

L62 ANSWER 33 OF 42 REGISTRY COPYRIGHT 2002 ACS

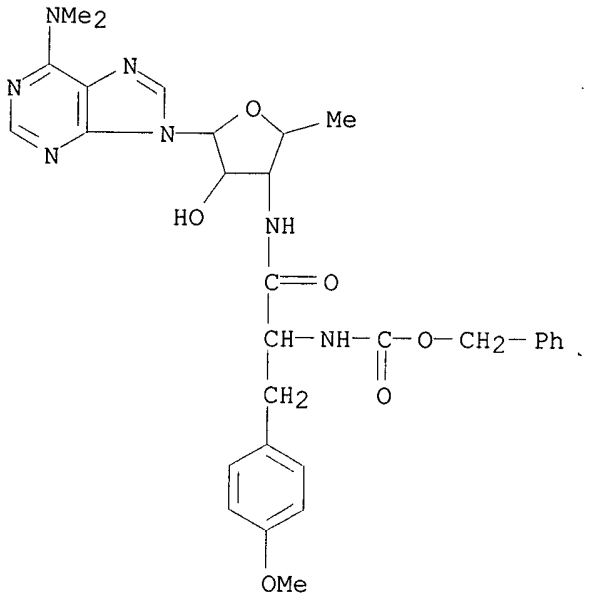
RN 50884-92-9 REGISTRY

CN Adenosine, 3',5'-dideoxy-3'-[[3-(4-methoxyphenyl)-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

MF C30 H35 N7 O6

LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 80:10760 Puromycin analogs. Synthesis and biological activity of 5'-deoxypuromycin and its aminonucleoside, 6-dimethylamino-9-(3'-amino-3',5'-dideoxy-.beta.-D-ribofuranosyl)purine. Almquist, Ronald G.; Vince, Robert (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 16(12), 1396 (English) 1973. CODEN: JMCMAR.

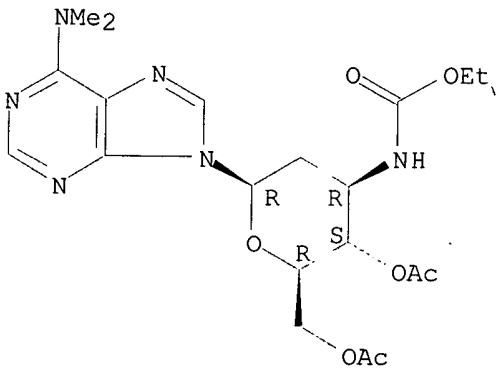
AB The 5'-hydroxyl of puromycin (I) [53-79-2] was not essential for inhibition of protein synthesis by I. Thus, 5'-deoxypuromycin [43157-40-0] was approx. twice as potent as I in inhibiting growth of Staphylococcus aureus and Escherichia coli in vitro. However, puromycin aminonucleoside [58-60-6], which lacked the amino acyl moiety, was cytotoxic to P388 mouse lymphoid leukemia cells in vitro at an LD50 of 8.1 .tim. 10-6M, whereas the corresponding 5'-deoxy deriv. 6-dimethylamino-9-(3'-amino-3',5'-dideoxy-.beta.-D-ribofuranosyl)purine (II) [43157-41-1] was inactive even at 40 times this concn. To synthesize 5'-deoxypuromycin, 1,2-O-isopropylidene-5-deoxy-.alpha.-D-xylofuranose [4152-79-8] was converted via the 3-keto and 3-oxime derivs. to the 3-amino sugar, which was N-acetylated, deblocked, converted to the 1,2-di-O-acetate, then to the 1-chloro sugar, condensed with 6-chloropurine [87-42-3] in the presence of Hg(CN)2, treated with aq. NHMe2, and hydrolyzed with Ba(OH)2 to yield II. Coupling of II with N-benzyloxycarbonyl-p-methoxyphenyl-L-alanine [17554-34-6] in the presence of dicyclohexylcarbodiimide and N-hydroxysuccinimide, followed by hydrogenolysis, yielded 5'-deoxypuromycin.

L62 ANSWER 34 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 39491-34-4 REGISTRY
CN 9H-Purin-6-amine, 9-[4,6-di-O-acetyl-2,3-dideoxy-3-[(ethoxycarbonyl)amino]-.beta.-D-arabino-hexopyranosyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 6-Dimethylamino-9-(4,6-di-O-acetyl-2,3-dideoxy-3-ethoxycarbonylamino-.beta.-D-arabino-hexopyranosyl)purine
FS STEREOSEARCH

Searched by: Mary Hale 308-4258 CM-1 12D16

MF C20 H28 N6 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

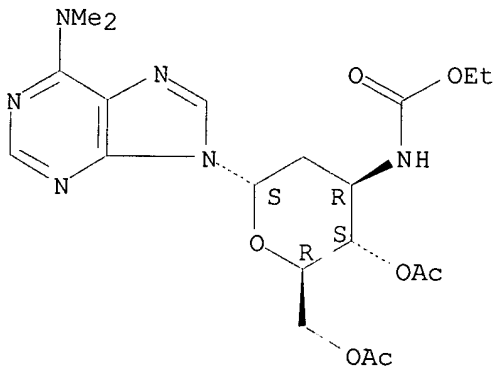
REFERENCE 1: 78:4464 Synthesis of some purine nucleosides from 4,6-di-O-acetyl-3-deoxy-3-(ethoxycarbonylamino)-D-glucal. Lourens, Gerhardus J.; Jordaan, A. (Natl. Chem. Res. Lab., Counc. Sci. Ind. Res., Pretoria, S. Afr.). J. Heterocycl. Chem., 9(5), 975-7 (English) 1972. CODEN: JHTCAD.

AB The acid catalyzed reaction of 4,o-di-O-acetyl-1.5-anhydro-3-deoxy-3-(ethoxycarbonylamino)-D-arabino-hex-1-enitol and 6-chloropurine in MeNO3 gave 6-chloro-9-(4',-o'-di-O-acetyl-2),3'-dideoxy-3'-ethoxycarbonylamino-.alpha.- and -.beta.-D-arabino-hexopyranosyl)purine. These were converted to the corresponding deblocked 6-dimethylaminopurine nucleosides by treatment with Me2NH in EtOH and then acetylation gave the resp. 4',o'-di-O-acetyl derivs. The anomeric assignments for the nucleosides were based on NMR spectral data.

L62 ANSWER 35 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 39491-33-3 REGISTRY
CN 9H-Purin-6-amine, 9-[4,6-di-O-acetyl-2,3-dideoxy-3-[(ethoxycarbonyl)amino]-.alpha.-D-arabino-hexopyranosyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H28 N6 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

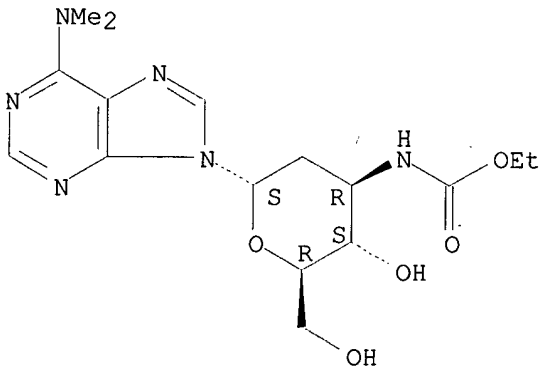
REFERENCE 1: 78:4464 Synthesis of some purine nucleosides from 4,6-di-O-acetyl-3-deoxy-3-(ethoxycarbonylamino)-D-glucal. Lourens, Gerhardus J.; Jordaan, A. (Natl. Chem. Res. Lab., Counc. Sci. Ind. Res., Pretoria, S. Afr.). J. Heterocycl. Chem., 9(5), 975-7 (English) 1972. CODEN: JHTCAD.

AB The acid catalyzed reaction of 4,o-di-O-acetyl-1.5-anhydro-3-deoxy-3-(ethoxycarbonylamino)-D-arabino-hex-1-enitol and 6-chloropurine in MeNO3 gave 6-chloro-9-(4',-o'-di-O-acetyl-2),3'-dideoxy-3'-ethoxycarbonylamino-.alpha.- and -.beta.-D-arabino-hexopyranosyl)purine. These were converted to the corresponding deblocked 6-dimethylaminopurine nucleosides by treatment with Me2NH in EtOH and then acetylation gave the resp. 4',o'-di-O-acetyl derivs. The anomeric assignments for the nucleosides were based on NMR spectral data.

L62 ANSWER 36 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 39491-32-2 REGISTRY
CN 9H-Purin-6-amine, 9-[2,3-dideoxy-3-[(ethoxycarbonyl)amino]-.alpha.-D-arabino-hexopyranosyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 6-Dimethylamino-9-(2,3-dideoxy-3-ethoxycarbonylamino-.alpha.-D-arabino-hexopyranosyl)purine
FS STEREOSEARCH
MF C16 H24 N6 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

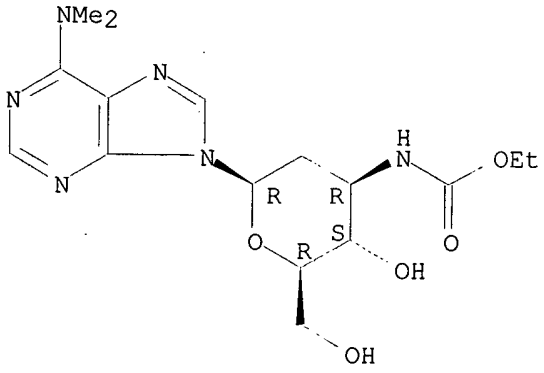
REFERENCE 1: 78:4464 Synthesis of some purine nucleosides from 4,6-di-O-acetyl-3-deoxy-3-(ethoxycarbonylamino)-D-glucal. Lourens, Gerhardus J.; Jordaan, A. (Natl. Chem. Res. Lab., Counc. Sci. Ind. Res., Pretoria, S. Afr.). J. Heterocycl. Chem., 9(5), 975-7 (English) 1972. CODEN: JHTCAD.

AB The acid catalyzed reaction of 4,o-di-O-acetyl-1.5-anhydro-3-deoxy-3-(ethoxycarbonylamino)-D-arabino-hex-1-enitol and 6-chloropurine in MeNO3 gave 6-chloro-9-(4',-o'-di-O-acetyl-2),3'-dideoxy-3'-ethoxycarbonylamino-.alpha.- and -.beta.-D-arabino-hexopyranosyl)purine. These were converted to the corresponding deblocked 6-dimethylaminopurine nucleosides by treatment with Me2NH in EtOH and then acetylation gave the resp. 4',o'-di-O-acetyl derivs. The anomeric assignments for the nucleosides were based on NMR spectral data.

L62 ANSWER 37 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 39491-31-1 REGISTRY
CN 9H-Purin-6-amine, 9-[2,3-dideoxy-3-[(ethoxycarbonyl)amino]-.beta.-D-arabino-hexopyranosyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 6-Dimethylamino-9-(2,3-dideoxy-3-ethoxycarbonylamino-.beta.-D-arabino-hexopyranosyl)purine
FS STEREOSEARCH
MF C16 H24 N6 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

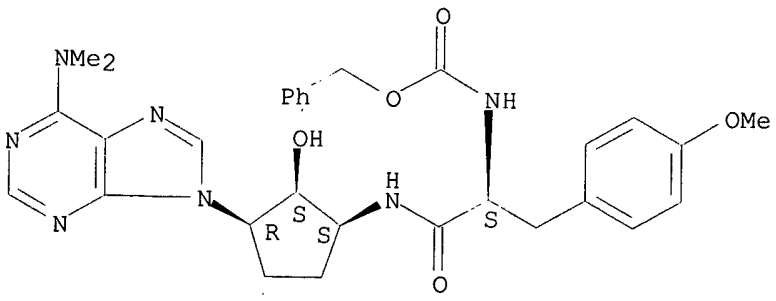
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 78:4464 Synthesis of some purine nucleosides from 4,6-di-O-acetyl-3-deoxy-3-(ethoxycarbonylamino)-D-glucal. Lourens, Gerhardus J.; Jordaan, A. (Natl. Chem. Res. Lab., Counc. Sci. Ind. Res., Pretoria, S. Afr.). J. Heterocycl. Chem., 9(5), 975-7 (English) 1972. CODEN: JHTCAD.

AB The acid catalyzed reaction of 4,o-di-O-acetyl-1.5-anhydro-3-deoxy-3-(ethoxycarbonylamino)-D-arabino-hex-1-enitol and 6-chloropurine in MeNO3 gave 6-chloro-9-(4',-o'-di-O-acetyl-2),3'-dideoxy-3'-ethoxycarbonylamino-.alpha.- and -.beta.-D-arabino-hexopyranosyl)purine. These were converted to the corresponding deblocked 6-dimethylaminopurine nucleosides by treatment with Me2NH in EtOH and then acetylation gave the resp. 4',o'-di-O-acetyl derivs. The anomeric assignments for the nucleosides were based on NMR spectral data.

L62 ANSWER 38 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 36341-60-3 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



Searched by: Mary Hale 308-4258 CM-1 12D16

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 82:58074 (+-)-9-.beta.-(3-.alpha.-Amino-2.alpha.-hydroxy cyclopentyl)-6-substituted-purines and derivatives. Vince, Robert (University of Minnesota). U.S. US 3825541 19740723, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1972-220890 19720126.

GI For diagram(s), see printed CA Issue.

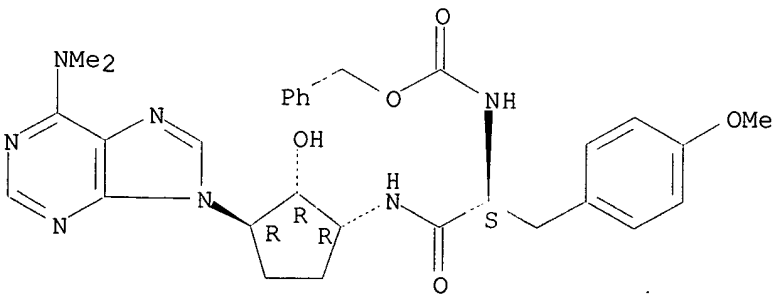
AB Pyromycin analogs (I and II) possessing bactericidal, antiprotozoan and anticancer activity were prepd. via coupling (.+-.)-9-[.beta.-(3.alpha.-amino-2.alpha.-hydroxy)cyclopentyl]-6-(dimethylamino)purine with N-benzyloxycarbonyl-p-methoxyphenyl-L-alanine. One isomer, assumed to be I, exhibited bactericidal activity equiv. to puromycin, whereas II was completely inactive.

REFERENCE 2: 76:122282 Synthesis and antimicrobial activity of a carbocyclic puromycin analog. 6-Dimethylamino-9-[R-[2R-hydroxy-3R-(p-methoxyphenyl-L-alanylamino)]cyclopentyl]purine. Daluge, Susan; Vince, Robert (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 15(2), 171-7 (English) 1972. CODEN: JMCMAR.

AB 6-Dimethylamino-9-[R-[2R-hydroxy-3R-(p-methoxyphenyl-L-alanylamino)]cyclopentyl]purine (I) [34597-43-8], a carbocyclic puromycin (II) [53-79-2] analog, was synthesized by condensing trans-3-amino-2-hydroxycyclopentanone ethylene ketal, prepd. from 2-cyclopentenone ethylene ketal, with 5-amino-4,6-dichloropyridine, followed by ring closure of the resulting pyrimidine with CH(OEt)3 to give trans-3-(6-chloro-9-purinyl)-2-hydroxycyclopentanone ethylene ketal, which was converted to its 6-(dimethylamino) deriv. The ketal was opened by heating with H2NOH.HCl at pH 1 affording trans-3-(6-dimethylamino-9-purinyl)-2-hydroxycyclopentanone oxime, which was converted to I via a multi-step synthesis. I exhibited antimicrobial activity comparable to that of II, but lacked the undesirable kidney damaging effects assocd. with II. The diastereoisomer of I was devoid of antimicrobial activity.

L62 ANSWER 39 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 36341-59-0 REGISTRY
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H35 N7 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



Searched by: Mary Hale 308-4258 CM-1 12D16

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 82:58074 (+-)-9-.beta.-(3-.alpha.-Amino-2.alpha.-hydroxy cyclopentyl)-6-substituted-purines and derivatives. Vince, Robert (University of Minnesota). U.S. US 3825541 19740723, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1972-220890 19720126.

GI For diagram(s), see printed CA Issue.

AB Pyromycin analogs (I and II) possessing bactericidal, antiprotozoan and anticancer activity were prepd. via coupling (.+-.)-9-[.beta.-(3.alpha.-amino-2.alpha.-hydroxy)cyclopentyl]-6-(dimethylamino)purine with N-benzyloxycarbonyl-p-methoxyphenyl-L-alanine. One isomer, assumed to be I, exhibited bactericidal activity equiv. to puromycin, whereas II was completely inactive.

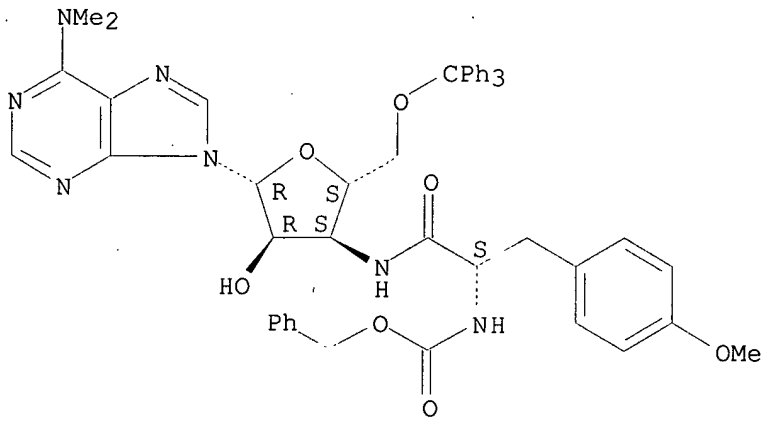
REFERENCE 2: 76:122282 Synthesis and antimicrobial activity of a carbocyclic puromycin analog. 6-Dimethylamino-9-[R-[2R-hydroxy-3R-(p-methoxyphenyl-L-alanylamino)]cyclopentyl]purine. Daluge, Susan; Vince, Robert (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 15(2), 171-7 (English) 1972. CODEN: JMCMAR.

AB 6-Dimethylamino-9-[R-[2R-hydroxy-3R-(p-methoxyphenyl-L-alanylamino)]cyclopentyl]purine (I) [34597-43-8], a carbocyclic puromycin (II) [53-79-2] analog, was synthesized by condensing trans-3-amino-2-hydroxycyclopentanone ethylene ketal, prepd. from 2-cyclopentenone ethylene ketal, with 5-amino-4,6-dichloropyridine, followed by ring closure of the resulting pyrimidine with CH(OEt)3 to give trans-3-(6-chloro-9-purinyl)-2-hydroxycyclopentanone ethylene ketal, which was converted to its 6-(dimethylamino) deriv. The ketal was opened by heating with H2NOH.HCl at pH 1 affording trans-3-(6-dimethylamino-9-purinyl)-2-hydroxycyclopentanone oxime, which was converted to I via a multi-step synthesis. I exhibited antimicrobial activity comparable to that of II, but lacked the undesirable kidney damaging effects assocd. with II. The diastereoisomer of I was devoid of antimicrobial activity.

L62 ANSWER 40 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 22852-14-8 REGISTRY
CN Adenosine, 3'-[.alpha.-(carboxyamino)-p-methoxyhydrocinnamamido]-3'-deoxy-N,N-dimethyl-5'-O-trityl-, benzyl ester, L- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C49 H49 N7 O7
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

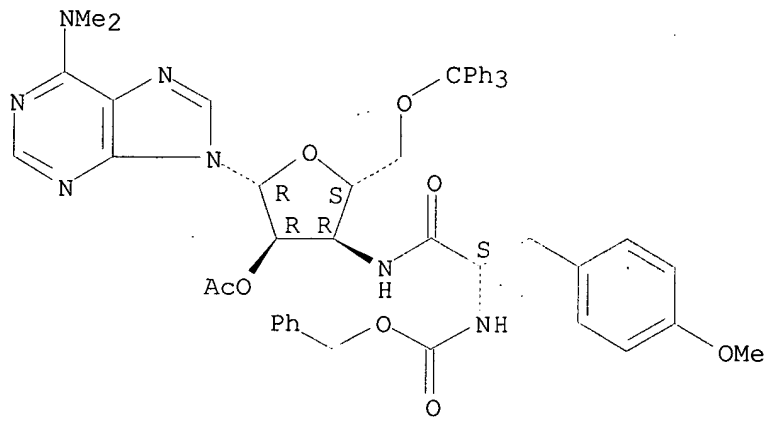
REFERENCE 1: 70:93232 Intramolecular acyl migration in adenosine derivatives. Neumann, Helmut; Shashoua, Victor E.; Sheehan, John C.; Rich, Alexander (Massachusetts Inst. of Technol., Cambridge, Mass., USA). Proc. Nat. Acad. Sci. U. S., 61(4), 1207-14 (English) 1968. CODEN: PNASA6.

AB Phenylalanylphenylalanine was formed from 2',3'-diphenylalanyl adenosine in aq. and non-aq. media. The order of this reaction was not established because of the complexity of the reaction products. The formation of the N-acetylpuromycin (I) from 2'-O-acetyl puromycin was a 1st-order reaction which probably proceeded via the formation of an intermediate complex. The transition state involved a nucleophilic attack by the electron pair of the amino group of puromycin onto the carbonyl of the acetyl group in the 2' OH position. The attack was catalyzed by a concomitant attack by a base on the amino group which aided in proton withdrawal. The reaction for the formation of I was unimol. and 1st-order only in the presence of a base such as diiso-propylethylamine (II). In the absence of II, the reaction probably had kinetics intermediate between 1st- and 2nd-order. The intermediate formed a quasi-6-membered ring.

L62 ANSWER 41 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 22768-42-9 REGISTRY
CN Adenosine, 3'-[.alpha.-(carboxyamino)-p-methoxyhydrocinnamamido]-3'-deoxy-N,N-dimethyl-5'-O-trityl-, benzyl ester, 2'-acetate, L- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C51 H51 N7 O8
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

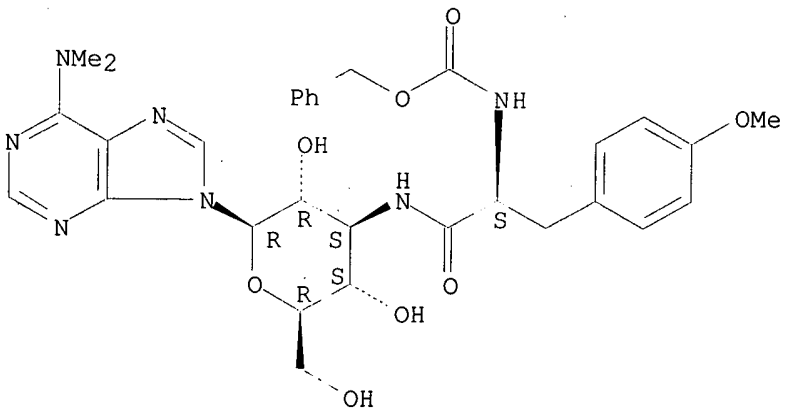
REFERENCE 1: 70:93232 Intramolecular acyl migration in adenosine derivatives. Neumann, Helmut; Shashoua, Victor E.; Sheehan, John C.; Rich, Alexander (Massachusetts Inst. of Technol., Cambridge, Mass., USA). Proc. Nat. Acad. Sci. U. S., 61(4), 1207-14 (English) 1968. CODEN: PNASA6.

AB Phenylalanylphenylalanine was formed from 2',3'-diphenylalanyl adenosine in aq. and non-aq. media. The order of this reaction was not established because of the complexity of the reaction products. The formation of the N-acetylpuromycin (I) from 2'-O-acetyl puromycin was a 1st-order reaction which probably proceeded via the formation of an intermediate complex. The transition state involved a nucleophilic attack by the electron pair of the amino group of puromycin onto the carbonyl of the acetyl group in the 2' OH position. The attack was catalyzed by a concomitant attack by a base on the amino group which aided in proton withdrawal. The reaction for the formation of I was unimol. and 1st-order only in the presence of a base such as diiso-propylethylamine (II). In the absence of II, the reaction probably had kinetics intermediate between 1st- and 2nd-order. The intermediate formed a quasi-6-membered ring.

L62 ANSWER 42 OF 42 REGISTRY COPYRIGHT 2002 ACS
RN 21017-00-5 REGISTRY
CN Adenine, 9-[3-[L-.alpha.-(carboxyamino)-p-methoxyhydrocinnamamido]-3-deoxy-.beta.-D-glucopyranosyl]-N,N-dimethyl-, benzyl ester (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H37 N7 O8
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 69:44159 Nucleosides. IV. Synthesis of a puromycin analog. Lichtenthaler, F. W.; Albrecht, H. P. (Tech. Hochsch. Darmstadt, Darmstadt, Ger.). Angew. Chem. Int. Ed. Engl., 7(6), 457-8 (English) 1968. CODEN: ACIEAY.

GI For diagram(s), see printed CA Issue.

AB 3-Deoxy-6-(dimethylamino)-9-[3-(X-substituted)-.beta.-D-glucopyranosyl]purines (I) are prepd. from 6-(dimethylamino)-9-(.beta.-D-ribofuranosyl)purine (II). II is treated with periodate to give a nucleoside dicarboxaldehyde, which is treated with MeNO2 in the presence of NaOMe to give I(X = NO2); I(X = NO2) is hydrogenated to give I(X = NH2) (III). III is treated with the mixed anhydride of ClCO2Et and L-p-MeO-C6H4CH2CH(NHCO2CH2Ph)CO2H to give I[X = p-MeOC6H4CH2CH(NH2)CONH].

=> fil caols; l62
'CAOLS' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'REGISTRY'
COMMAND STACK INTERRUPTED. ENTER "DISPLAY HISTORY"
TO SEE WHICH COMMANDS WERE EXECUTED.

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> fil caol; l62

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1076.54	1734.76
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-23.60	-47.61

FILE 'CAOLD' ENTERED AT 14:05:11 ON 29 APR 2002

Searched by: Mary Hale 308-4258 CM-1 12D16

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

L62 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s l62
L63 1 L62

=> d

L63 ANSWER 1 OF 1 CAOLD COPYRIGHT 2002 ACS
AN CA52:2936i CAOLD
TI aminoglycosidopurines
PA American Cyanamid Co.
DT Patent

PATENT NO.	KIND	DATE
GB 782440		

IT 72-94-6 2504-55-4 6044-48-0 6161-07-5 6997-08-6 21299-78-5
51236-40-9 92870-26-3 99672-42-1 100245-75-8 108761-17-7
109104-86-1 109366-69-0 109514-96-7 109514-98-9 109698-68-2
110115-47-4 110274-27-6 **112072-20-5** 112718-09-9 113134-88-6
114863-81-9 115101-58-1 115120-96-2 116606-84-9 117273-79-7 119622-11-6
120207-56-9 120945-44-0 120969-31-5 121970-12-5 121970-21-6 121990-69-0
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132129-30-7 133102-30-4 133498-33-6 133498-34-7 133498-35-8 133498-36-9

=> fil caplus;s l62

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.95	1735.71

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-47.61

FILE 'CAPLUS' ENTERED AT 14:05:26 ON 29 APR 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Searched by: Mary Hale 308-4258 CM-1 12D16

FILE COVERS 1907 - 29 Apr 2002 VOL 136 ISS 18
FILE LAST UPDATED: 28 Apr 2002 (20020428/ED)

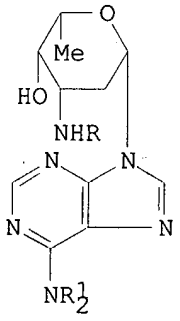
This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

L64 20 L62

=> d 11-20 cbib abs hitstr

L64 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2002 ACS
1977:485194 Document No. 87:85194 Synthesis of some purine and pyrimidine nucleosides of 3-amino-2,3,6-trideoxy-L-lyxo-hexopyranose (daunosamine). Lazzari, Ettore; Vigevani, Aristide; Arcamone, Federico (Res. Lab., Farmitalia, Milan, Italy). Carbohydr. Res., 56(1), 35-42 (English) 1977. CODEN: CRBRAT.
GI

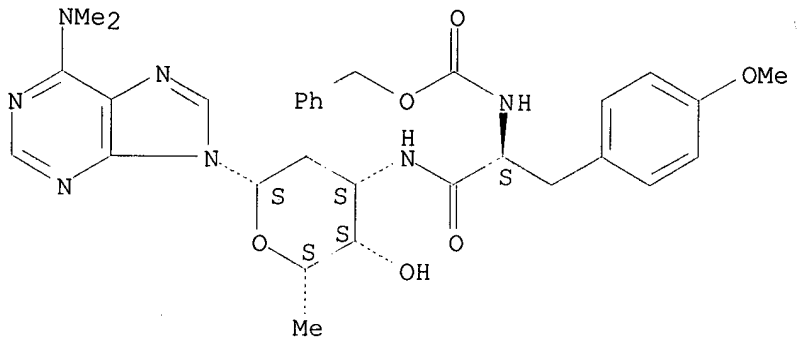


I

AB The daunosaminyl analog of puromycin and the nucleoside derivs. of 6-dimethylaminopurine, thymine, and cytosine were prepd. by melting the protected daunosamine with the protected base in vacuo. Thus, I (R = R1 = H) was prepd. by condensation of N,O-ditrifluoroacetyl-.alpha.-daunosaminyl chloride with either N6-benzoyl-9-chloromercuriadenine or N6-benzoyladenine. Coupling of I (R = H, R1 = Me) with PhCH2O2C-Tyr(OMe)-OH followed by hydrogenolysis gave the daunosaminyl analog I (R = 4-MeOC6H4CH2CH(NH2)CO, R1 = Me) of puromycin.
IT **63622-03-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenolysis of)
RN 63622-03-7 CAPLUS
CN 9H-Purin-6-amine, N,N-dimethyl-9-[2,3,6-trideoxy-3-[[3-(4-methoxyphenyl)-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-.beta.-L-lyxo-hexopyranosyl]-, (S)- (9CI) (CA INDEX NAME)

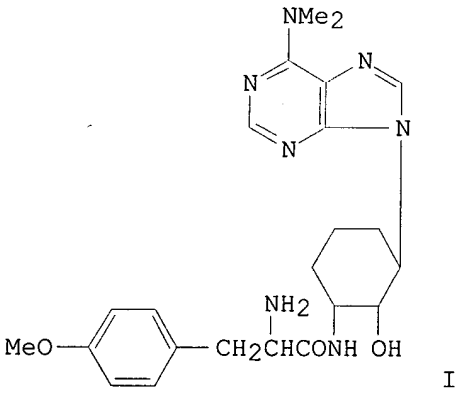
Searched by: Mary Hale 308-4258 CM-1 12D16

Absolute stereochemistry.



L64 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2002 ACS
1977:463341 Document No. 87:63341 Synthesis of cyclohexyl carbocyclic puromycin and its inhibition of protein synthesis. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 20(7), 930-4 (English) 1977. CODEN: JMCMAR.

GI



I

AB Four title compds., 6-dimethylamino-9-[(R)-[2(R)-hydroxy-3(R)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine (I) [62854-09-5], 6-dimethylamino-9-[(S)-[2(S)-hydroxy-3(S)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-90-9], 6-dimethylamino-9-[(R)-[2(R)-hydroxy-3(S)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-87-4], and 6-dimethylamino-9-[(S)-[2(S)-hydroxy-3(R)-(p-methoxyphenyl-L-alanylamino)]cyclohexyl]purine [62928-91-0], were prepd. Of the above compds. and 2 trans-cyclopentyl carbocyclic puromycin analogs, all but I were inactive at 10-3 M as inhibitors of poly(U,C)-directed L-[14C]poly(phenylalanine) formation in an Escherichia coli cell-free ribosome system. I had a 45-fold lower activity than puromycin [53-79-2] in the same system in comparisons of 50% inhibition concns. Apparently, max. activity of puromycin analogs is obtained when the purine moiety, amino acid, and hydroxyl group are oriented about a 5-membered ring. The amino acid and hydroxyl group must be in a cis orientation, and the abs. stereochem. of the parent antibiotic must be conserved.

IT **62854-19-7P 62960-65-0P 62989-86-0P**

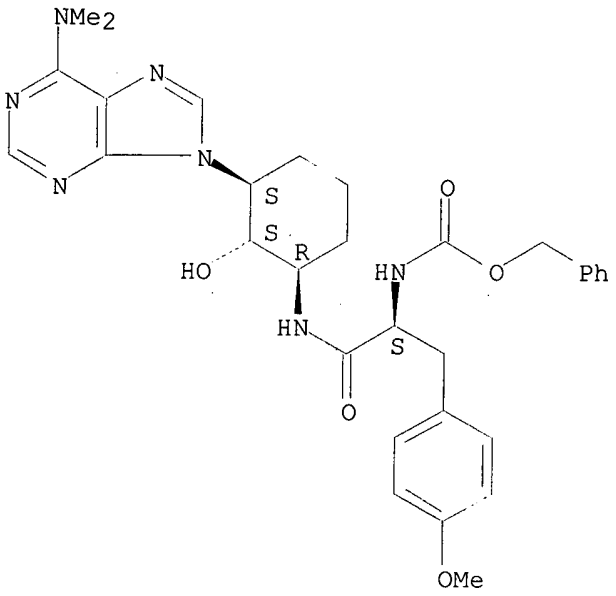
Searched by: Mary Hale 308-4258 CM-1 12D16

RL: RCT (Reactant); PREP (Preparation)
(prepn. and hydrogenolysis of)

RN 62854-19-7 CAPLUS

CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclohexyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.beta.,3.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

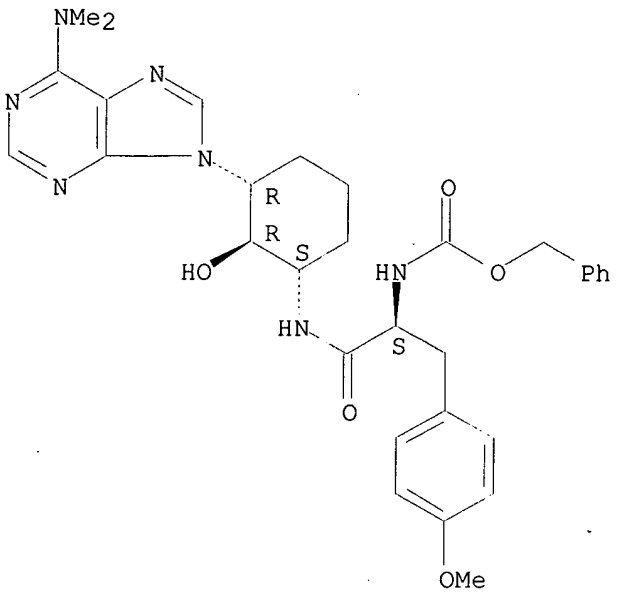


RN 62960-65-0 CAPLUS

CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclohexyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.beta.,3.alpha.]]- (9CI) (CA INDEX NAME)

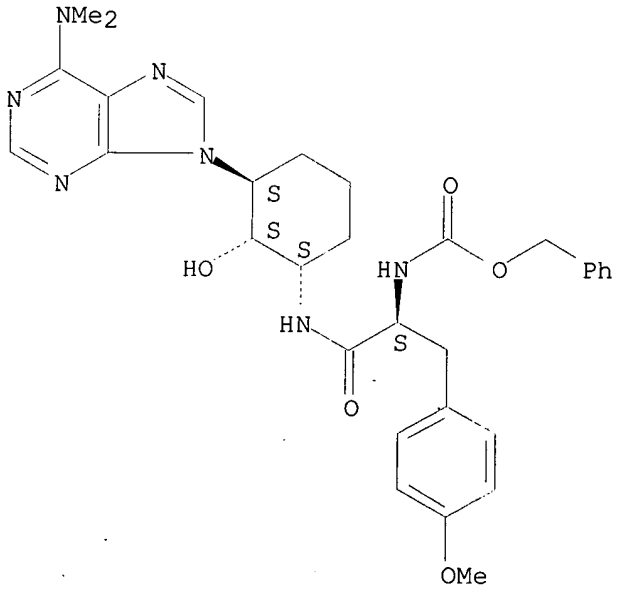
Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



RN 62989-86-0 CAPLUS
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclohexyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L64 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2002 ACS
1975:58074 Document No. 82:58074 (+-)-9-.beta.-(3-.alpha.-Amino-2.alpha.-hydroxy cyclopentyl)-6-substituted-purines and derivatives. Vince, Robert (University of Minnesota). U.S. US 3825541 19740723, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1972-220890 19720126.
GI For diagram(s), see printed CA Issue.

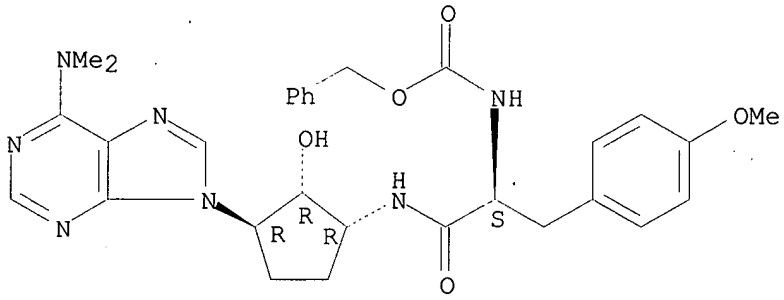
Searched by: Mary Hale 308-4258 CM-1 12D16

AB Pyromycin analogs (I and II) possessing bactericidal, antiprotozoan and anticancer activity were prepd. via coupling (.+-.)-9-[.beta.-(3.alpha.-amino-2.alpha.-hydroxy)cyclopentyl]-6-(dimethylamino)purine with N-benzyloxycarbonyl-p-methoxyphenyl-L-alanine. One isomer, assumed to be I, exhibited bactericidal activity equiv. to puromycin, whereas II was completely inactive.

IT **36341-59-0P 36341-60-3P 54700-35-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

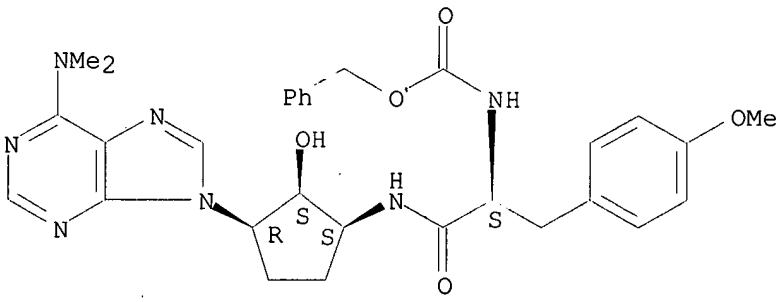
RN 36341-59-0 CAPLUS
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 36341-60-3 CAPLUS
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.alpha.]]- (9CI) (CA INDEX NAME)

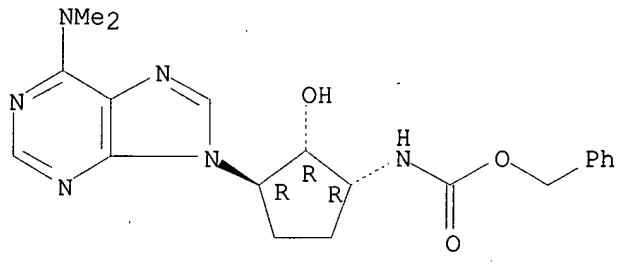
Absolute stereochemistry.



RN 54700-35-5 CAPLUS
CN Carbamic acid, [3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]-, phenylmethyl ester, (1.alpha.,2.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



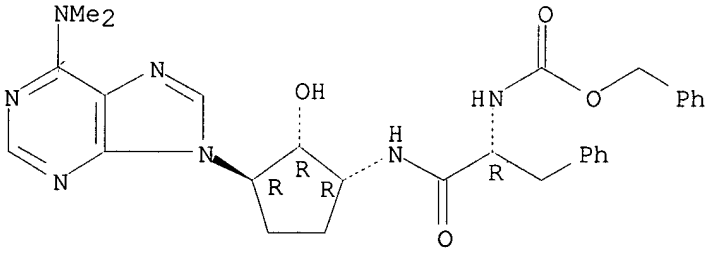
L64 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2002 ACS
1974:515149 Document No. 81:115149 Puromycin analogs. Ribosomal binding with diastereomeric carbocyclic puromycin analogs. Vince, Robert; Daluge, Susan (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 17(6), 578-83 (English) 1974. CODEN: JMCMAR.

AB Of 7 title compds. prepd. and found active in the inhibition of poly-UC-directed polyphenylalanine formation in an Escherichia coli cell-free system, 6-(dimethylamino)-9-[(R)-[(2R)-hydroxy-(3R)-(L-phenylalanylamino)]cyclopentyl]purine (I) [52661-26-4] gave 98.6% inhibition at 10-4M. I was prepd. from 3-acetamidocyclopentene [52661-16-2] by epoxidn., opening of the epoxide with NaN3 [26628-22-8], followed by redn. to the azido alc., resoln. via tartrate formation, introduction of the purine moiety, and coupling with the amino acid. The relation of structure of the various aminoacyl analogs to activity was discussed.

IT **52691-27-7 52691-28-8 52691-29-9**
RL: RCT (Reactant)
(hydrogenolysis of)

RN 52691-27-7 CAPLUS
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, [1R-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

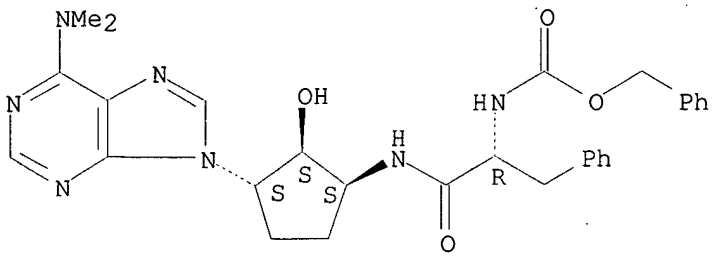
Absolute stereochemistry.



RN 52691-28-8 CAPLUS
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, [1S-[1.alpha.(S*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

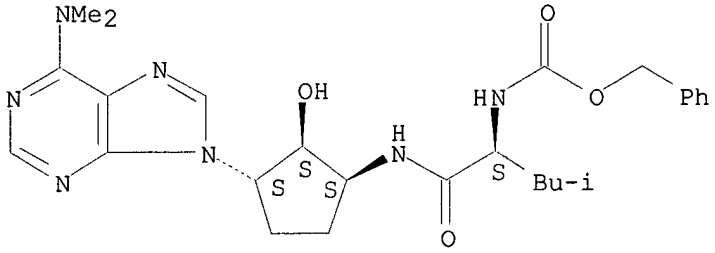
Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



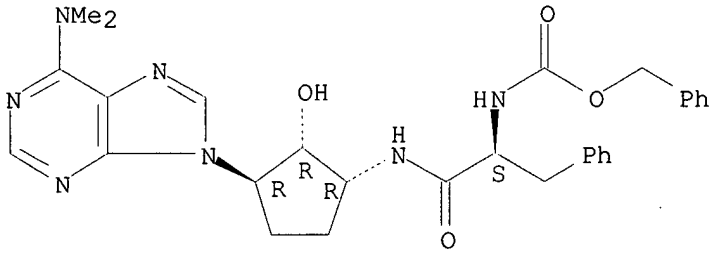
RN 52691-29-9 CAPLUS
CN Carbamic acid, [1-[[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **52661-23-1P 52661-24-2P 52661-25-3P 52691-26-6P**
RL: PREP (Preparation)
(prepn. of)
RN 52661-23-1 CAPLUS
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

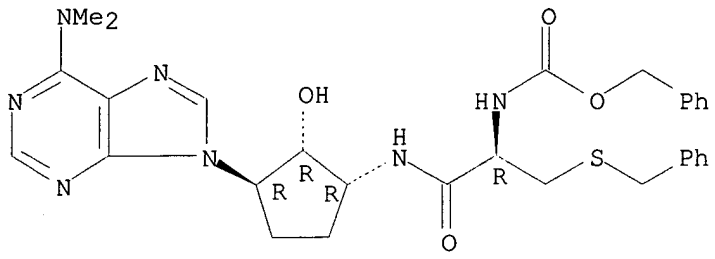
Absolute stereochemistry.



RN 52661-24-2 CAPLUS
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-[[(phenylmethyl)thio]methyl]ethyl]-, phenylmethyl ester, [1R-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

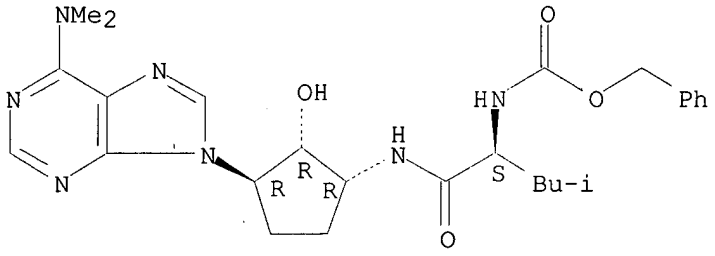
Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



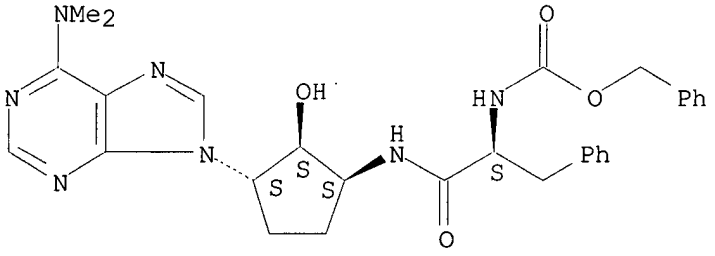
RN 52661-25-3 CAPLUS
CN Carbamic acid, [1-[[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 52691-26-6 CAPLUS
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L64 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2002 ACS
1974:108480 Document No. 80:108480 Unconventional nucleotide analogs. XI. Synthesis of a nonsaccharidal analog of puromycin. Kaspersen, Frans M.; Bieraugel, Hans; Pandit, Upendra K. (Org. Chem. Lab., Univ. Amsterdam, Amsterdam, Neth.). Heterocycles, 2(1), 15-19 (English) 1974. CODEN: HTCYAM.
GI For diagram(s), see printed CA Issue.
AB The title puromycin analog (I), of interest because of analogy to nucleo-peptide models, is prepd. Thus, (-)-4-hydroxy-L-proline was converted to II which on treatment with 5-amino-4,6-dichloropyrimidine followed by ring closure [(EtO)3CH] gave III (R = Cl, R1 = tosyl). Reaction of this with Me2NH and detosylation gave III (R = NMe2, R1 = H). Coupling of this with Cbz N-protected 4-MeOC6H4CH2CH(NH2)-CO2H gave, after

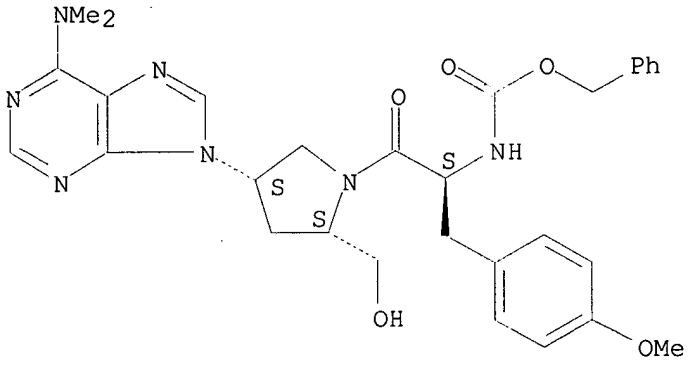
removal of the Cbz group, I.

IT **51846-78-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 51846-78-7 CAPLUS

CN Carbamic acid, [2-[4-[6-(dimethylamino)-9H-purin-9-yl]-2-(hydroxymethyl)-1-pyrrolidinyl]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [2S-[1(R*),2.alpha.,4.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L64 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2002 ACS

1974:10760 Document No. 80:10760 Puromycin analogs. Synthesis and biological activity of 5'-deoxypuromycin and its aminonucleoside, 6-dimethylamino-9-(3'-amino-3',5'-dideoxy-.beta.-D-ribofuranosyl)purine. Almquist, Ronald G.; Vince, Robert (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 16(12), 1396 (English) 1973. CODEN: JMCMAR.

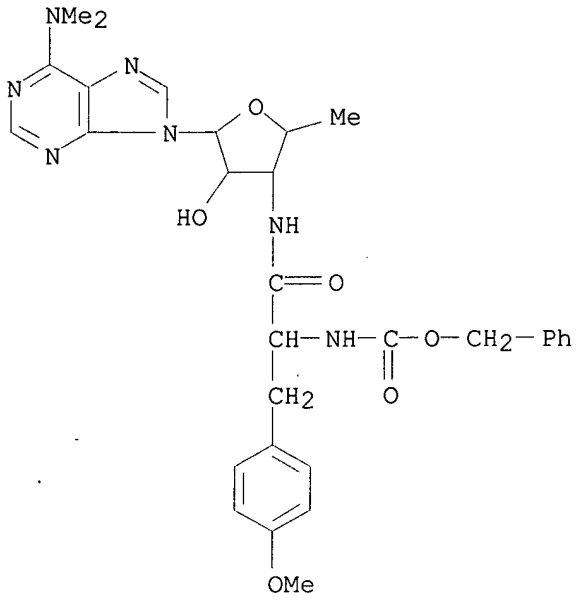
AB The 5'-hydroxyl of puromycin (I) [53-79-2] was not essential for inhibition of protein synthesis by I. Thus, 5'-deoxypuromycin [43157-40-0] was approx. twice as potent as I in inhibiting growth of Staphylococcus aureus and Escherichia coli in vitro. However, puromycin aminonucleoside [58-60-6], which lacked the amino acyl moiety, was cytotoxic to P388 mouse lymphoid leukemia cells in vitro at an LD50 of 8.1 .tim. 10-6M, whereas the corresponding 5'-deoxy deriv. 6-dimethylamino-9-(3'-amino-3',5'-dideoxy-.beta.-D-ribofuranosyl)purine (II) [43157-41-1] was inactive even at 40 times this concn. To synthesize 5'-deoxypuromycin, 1,2-O-isopropylidene-5-deoxy-.alpha.-D-xylofuranose [4152-79-8] was converted via the 3-keto and 3-oxime derivs. to the 3-amino sugar, which was N-acetylated, deblocked, converted to the 1,2-di-O-acetate, then to the 1-chloro sugar, condensed with 6-chloropurine [87-42-3] in the presence of Hg(CN)2, treated with aq. NHMe2, and hydrolyzed with Ba(OH)2 to yield II. Coupling of II with N-benzyloxycarbonyl-p-methoxyphenyl-L-alanine [17554-34-6] in the presence of dicyclohexylcarbodiimide and N-hydroxysuccinimide, followed by hydrogenolysis, yielded 5'-deoxypuromycin.

IT **50884-92-9P**
RL: PREP (Preparation)
(prepn. of)

RN 50884-92-9 CAPLUS

CN Adenosine, 3',5'-dideoxy-3'-[[3-(4-methoxyphenyl)-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16



L64 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2002 ACS

1973:4464 Document No. 78:4464 Synthesis of some purine nucleosides from 4,6-di-O-acetyl-3-deoxy-3-(ethoxycarbonylamino)-D-glucal. Lourens, Gerhardus J.; Jordaan, A. (Natl. Chem. Res. Lab., Counc. Sci. Ind. Res., Pretoria, S. Afr.). J. Heterocycl. Chem., 9(5), 975-7 (English) 1972. CODEN: JHTCAD.

AB The acid catalyzed reaction of 4,o-di-O-acetyl-1.5-anhydro-3-deoxy-3-(ethoxycarbonylamino)-D-arabino-hex-1-enitol and 6-chloropurine in MeNO3 gave 6-chloro-9-(4',-o'-di-O-acetyl-2),3'-dideoxy-3'-ethoxycarbonylamino-.alpha.- and -.beta.-D-arabino-hexopyranosyl)purine. These were converted to the corresponding deblocked 6-dimethylaminopurine nucleosides by treatment with Me2NH in EtOH and then acetylation gave the resp. 4',o'-di-O-acetyl derivs. The anomeric assignments for the nucleosides were based on NMR spectral data.

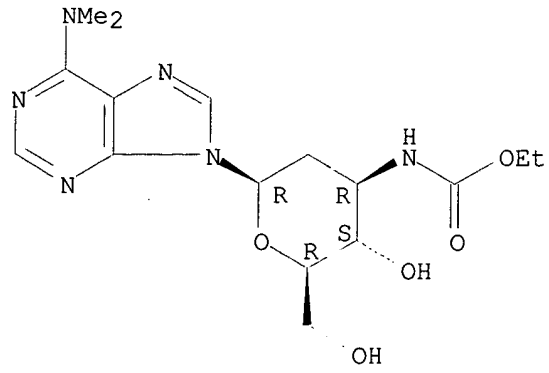
IT **39491-31-1P 39491-32-2P 39491-33-3P**
39491-34-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 39491-31-1 CAPLUS

CN 9H-Purin-6-amine, 9-[2,3-dideoxy-3-[(ethoxycarbonyl)amino]-.beta.-D-arabino-hexopyranosyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

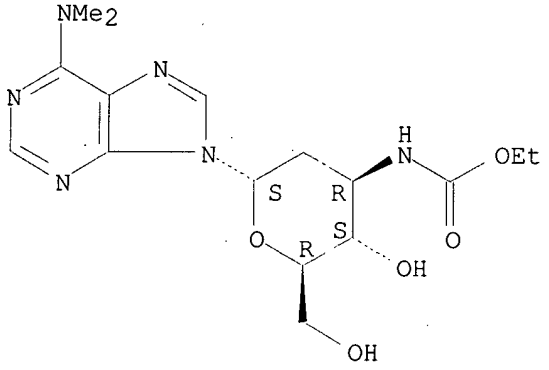
Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



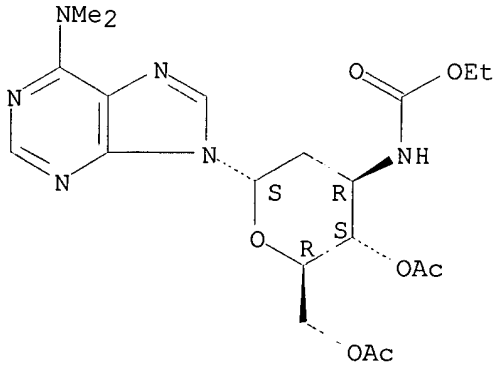
RN 39491-32-2 CAPLUS
CN 9H-Purin-6-amine, 9-[2,3-dideoxy-3-[(ethoxycarbonyl)amino]-.alpha.-D-arabino-hexopyranosyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 39491-33-3 CAPLUS
CN 9H-Purin-6-amine, 9-[4,6-di-O-acetyl-2,3-dideoxy-3-[(ethoxycarbonyl)amino]-.alpha.-D-arabino-hexopyranosyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

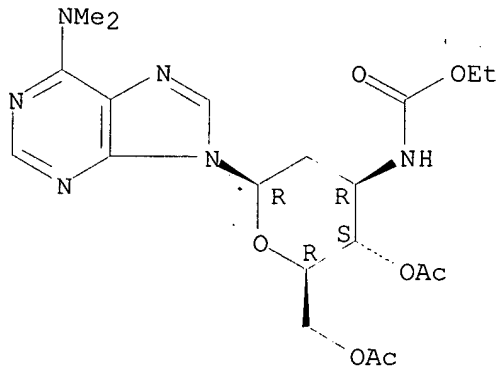
Absolute stereochemistry.



RN 39491-34-4 CAPLUS
CN 9H-Purin-6-amine, 9-[4,6-di-O-acetyl-2,3-dideoxy-3-[(ethoxycarbonyl)amino]-.beta.-D-arabino-hexopyranosyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

Absolute stereochemistry.



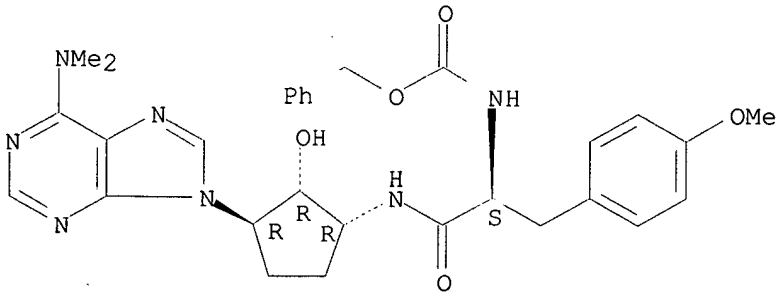
L64 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2002 ACS
1972:122282 Document No. 76:122282 Synthesis and antimicrobial activity of a carbocyclic puromycin analog. 6-Dimethylamino-9-[R-[2R-hydroxy-3R-(p-methoxyphenyl-L-alanylamino)]cyclopentyl]purine. Daluge, Susan; Vince, Robert (Coll. Pharm., Univ. Minnesota, Minneapolis, Minn., USA). J. Med. Chem., 15(2), 171-7 (English) 1972. CODEN: JMCMAR.

AB 6-Dimethylamino-9-[R-[2R-hydroxy-3R-(p-methoxyphenyl-L-alanylamino)]cyclopentyl]purine (I) [34597-43-8], a carbocyclic puromycin (II) [53-79-2] analog, was synthesized by condensing trans-3-amino-2-hydroxycyclopentanone ethylene ketal, prepd. from 2-cyclopentenone ethylene ketal, with 5-amino-4,6-dichloropyridine, followed by ring closure of the resulting pyrimidine with CH(OEt)3 to give trans-3-(6-chloro-9-purinyl)-2-hydroxycyclopentanone ethylene ketal, which was converted to its 6-(dimethylamino) deriv. The ketal was opened by heating with H2NOH.HCl at pH 1 affording trans-3-(6-dimethylamino-9-purinyl)-2-hydroxycyclopentanone oxime, which was converted to I via a multi-step synthesis. I exhibited antimicrobial activity comparable to that of II, but lacked the undesirable kidney damaging effects assocd. with II. The diastereoisomer of I was devoid of antimicrobial activity.

IT **36341-59-0P 36341-60-3P**
RL: PREP (Preparation)
(prepn. of)

RN 36341-59-0 CAPLUS
CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1R-[1.alpha.(S*),2.alpha.,3.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

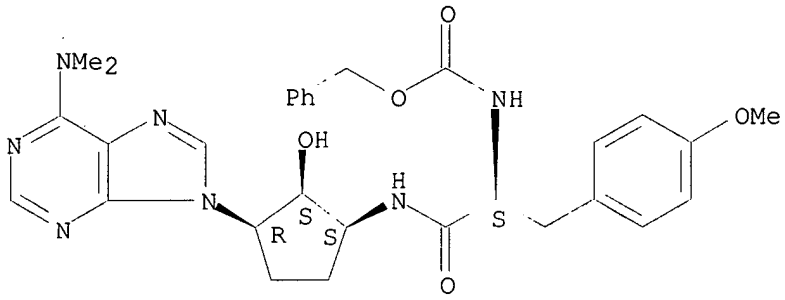


RN 36341-60-3 CAPLUS

Searched by: Mary Hale 308-4258 CM-1 12D16

CN Carbamic acid, [2-[[3-[6-(dimethylamino)-9H-purin-9-yl]-2-hydroxycyclopentyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, [1S-[1.alpha.(R*),2.alpha.,3.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L64 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2002 ACS

1969:93232 Document No. 70:93232 Intramolecular acyl migration in adenosine derivatives. Neumann, Helmut; Shashoua, Victor E.; Sheehan, John C.; Rich, Alexander (Massachusetts Inst. of Technol., Cambridge, Mass., USA). Proc. Nat. Acad. Sci. U. S., 61(4), 1207-14 (English) 1968. CODEN: PNASA6.

AB Phenylalanylphenylalanine was formed from 2',3'-diphenylalanyl adenosine in aq. and non-aq. media. The order of this reaction was not established because of the complexity of the reaction products. The formation of the N-acetylpuromycin (I) from 2'-O-acetyl puromycin was a 1st-order reaction which probably proceeded via the formation of an intermediate complex. The transition state involved a nucleophilic attack by the electron pair of the amino group of puromycin onto the carbonyl of the acetyl group in the 2' OH position. The attack was catalyzed by a concomitant attack by a base on the amino group which aided in proton withdrawal. The reaction for the formation of I was unimol. and 1st-order only in the presence of a base such as diiso-propylethylamine (II). In the absence of II, the reaction probably had kinetics intermediate between 1st- and 2nd-order. The intermediate formed a quasi-6-membered ring.

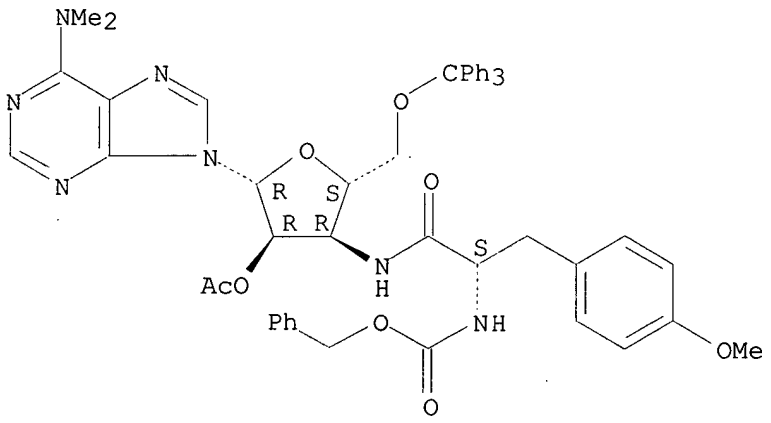
IT **22768-42-9P 22852-14-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 22768-42-9 CAPLUS

CN Adenosine, 3'-[.alpha.-(carboxyamino)-p-methoxyhydrocinnamamido]-3'-deoxy-N,N-dimethyl-5'-O-trityl-, benzyl ester, 2'-acetate, L- (8CI) (CA INDEX NAME)

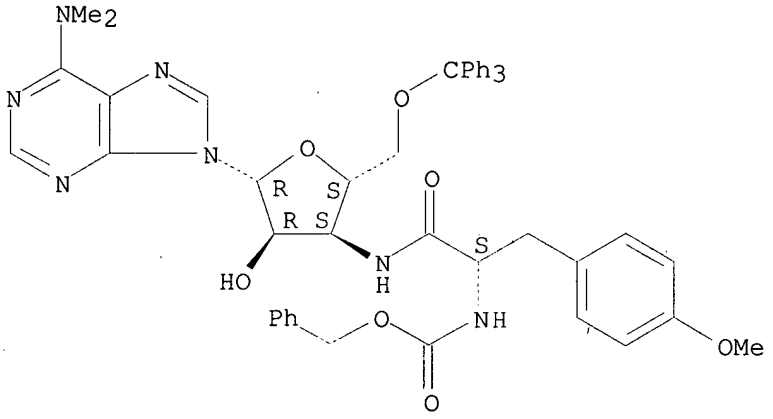
Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



RN 22852-14-8 CAPLUS
CN Adenosine, 3'-[.alpha.-(carboxyamino)-p-methoxyhydrocinnamamido]-3'-deoxy-N,N-dimethyl-5'-O-trityl-, benzyl ester, L- (8CI) (CA INDEX NAME)

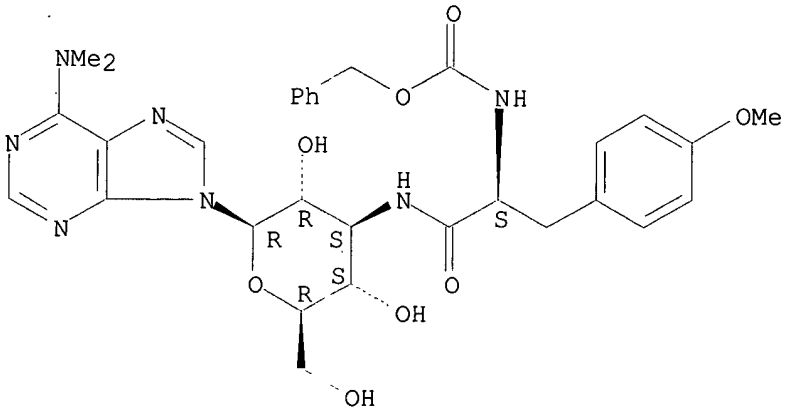
Absolute stereochemistry.



L64 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2002 ACS
1968:444159 Document No. 69:44159 Nucleosides. IV. Synthesis of a puromycin analog. Lichtenthaler, F. W.; Albrecht, H. P. (Tech. Hochsch. Darmstadt, Darmstadt, Ger.). Angew. Chem. Int. Ed. Engl., 7(6), 457-8 (English) 1968. CODEN: ACIEAY.
GI For diagram(s), see printed CA Issue.
AB 3-Deoxy-6-(dimethylamino)-9-[3-(X-substituted)-.beta.-D-glucopyranosyl]purines (I) are prepd. from 6-(dimethylamino)-9-(.beta.-D-ribofuranosyl)purine (II). II is treated with periodate to give a nucleoside dicarboxaldehyde, which is treated with MeNO2 in the presence of NaOMe to give I(X = NO2); I(X = NO2) is hydrogenated to give I(X = NH2) (III). III is treated with the mixed anhydride of ClCO2Et and L-p-MeO-C6H4CH2CH(NHCO2CH2Ph)CO2H to give I[X = p-MeOC6H4CH2CH(NH2)CONH].
IT **21017-00-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 21017-00-5 CAPLUS
CN Adenine, 9-[3-[L-.alpha.-(carboxyamino)-p-methoxyhydrocinnamamido]-3-deoxy-.beta.-D-glucopyranosyl]-N,N-dimethyl-, benzyl ester (8CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

Absolute stereochemistry.



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	44.29	1780.00

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.20	-53.81

STN INTERNATIONAL LOGOFF AT 14:05:54 ON 29 APR 2002

Searched by: Mary Hale 308-4258 CM-1 12D16

Beach
989348

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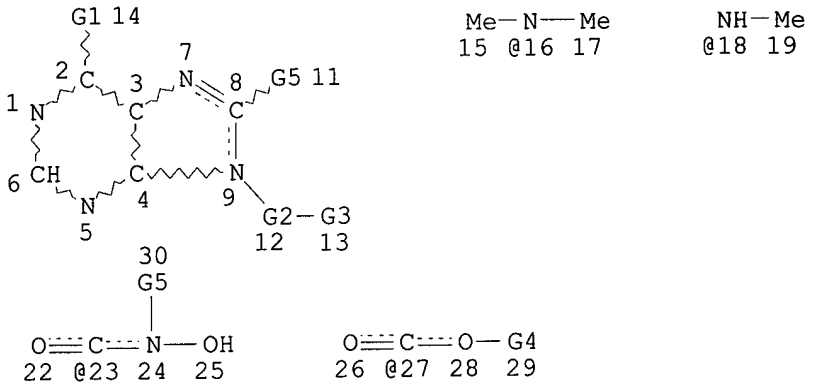

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VAR G4=H/C
VAR G5=H/ME
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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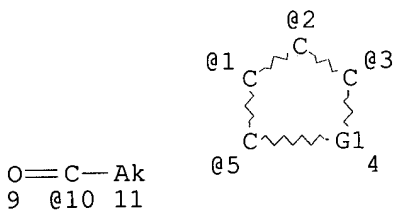
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L16 STR



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VPA 6-3/2/1/5 U
NODE ATTRIBUTES:
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GGCAT IS LOC AT 11
DEFAULT ECLEVEL IS LIMITED

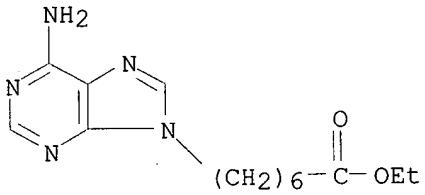
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

Searched by: Mary Hale 308-4258 CM-1 12D16

L17 SCR 1842 OR 2021 OR 2016 OR 2127 OR 1929 OR 2039 OR 2043
L24 46 SEA FILE=REGISTRY SSS FUL L15 NOT L16
L25 17 SEA FILE=REGISTRY SUB=L24 SSS FUL L17
L26 29 SEA FILE=REGISTRY ABB=ON PLU=ON L24 NOT L25

L26 ANSWER 1 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 359865-38-6 REGISTRY
CN 9H-Purine-9-heptanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H21 N5 O2
SR CA
LC STN Files: CA, CAPLUS



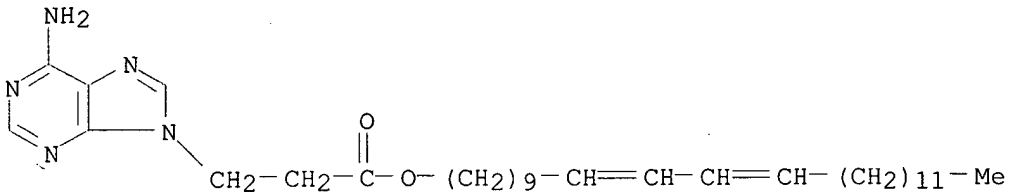
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:238179 Polymethylene derivatives of nucleic bases with .omega.-functional groups: II. Adenine and hypoxanthine derivatives. Makinsky, A. A.; Kritzyn, A. M.; Ul'yanova, E. A.; Zakharova, O. D.; Bugreev, D. V.; Nevinsky, G. A. (Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, 119991, Russia). Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya), 27(3), 167-172 (English) 2001. CODEN: RJBCET. ISSN: 1068-1620. Publisher: MAIK Nauka/Interperiodica.
AB N9-Polymethylene derivs. of adenine and hypoxanthine with various functional groups in the .omega.-position of the alkyl substituent were synthesized. Their physicochem. properties and effect on the HIV reverse transcriptase and DNA topoisomerase I were studied.

L26 ANSWER 2 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 353485-60-6 REGISTRY
CN 9H-Purine-9-propanoic acid, 6-amino-, 10,12-pentacosadienyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C33 H55 N5 O2
SR CA
LC STN Files: CA, CAPLUS

Searched by: Mary Hale 308-4258 CM-1 12D16



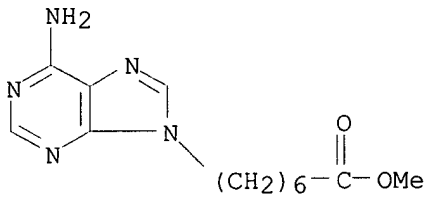
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:163889 Molecular assemblies based on DNA-mimetics: Effect of monolayer matrix on photopolymerization of diacetylene-containing nucleobase monolayers. Ijiro, Kuniharu; Matsumoto, Jin; Shimomura, Masatsugu (Research Institute for Electronic Science, Hokkaido University, Sapporo, 060-0812, Japan). Studies in Surface Science and Catalysis, 132(Proceedings of the International Conference on Colloid and Surface Science, 2000), 481-484 (English) 2001. CODEN: SSCTDM. ISSN: 0167-2991. Publisher: Elsevier Science B.V..

AB Pressure-area isotherm of a ternary component monolayer of nucleobase amphiphiles, diacetylene-contg. adenine and thymine amphiphiles (DA-Ade and DA-Thy), and octadecylcytosine (C18-Cyt), on the aq. dT30 subphase was changed by addn. of poly(G) into the subphase. Photopolymn. of the ternary monolayers on the aq. dT30 soln. was almost identical with that of a binary monolayer (DA-Ade/DA-Thy) on the same subphase. Addn. of poly(G) into the subphase suppressed photopolymn. of the ternary monolayer. Since the DA-Ade/DA-Thy pairs complexed with dT30 were clustered in the C18-Cyt matrix, both intra- and inter-complex polymn. were occurred on the dT30 subphase. The inter-complex polymn. was restrained by mixing with C18-Cyt / poly(G) matrix.

L26 ANSWER 3 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 326797-77-7 REGISTRY
CN 9H-Purine-9-heptanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H19 N5 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

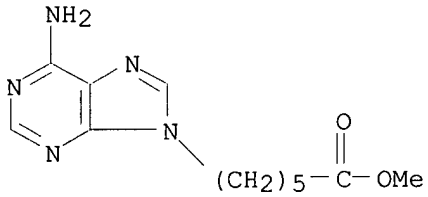
REFERENCE 1: 134:178789 Synthesis of purine derivatives of potential immunomodulatory activity. Pini, E.; Rossi, E.; Ferraris, P. Cornaglia;

Searched by: Mary Hale 308-4258 CM-1 12D16

Stradi, R. (Instituto di Chimica Organica-Facolta di Farmacia-Universita degli Studi di Milano, Milan, 20133, Italy). Bollettino Chimico Farmaceutico, 139(3), 107-113 (English) 2000. CODEN: BCFAAI. ISSN: 0006-6648. Publisher: Societa Editoriale Farmaceutica.

AB Moving from the interest as immunomodulatory agent of ST789 was studied the synthesis of series of N9-alkylated hypoxanthine and adenine. The synthesis and the chem. phys. properties of these derivs. are here described.

L26 ANSWER 4 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 326797-76-6 REGISTRY
CN 9H-Purine-9-hexanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H17 N5 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:178789 Synthesis of purine derivatives of potential immunomodulatory activity. Pini, E.; Rossi, E.; Ferraris, P. Cornaglia; Stradi, R. (Instituto di Chimica Organica-Facolta di Farmacia-Universita degli Studi di Milano, Milan, 20133, Italy). Bollettino Chimico Farmaceutico, 139(3), 107-113 (English) 2000. CODEN: BCFAAI. ISSN: 0006-6648. Publisher: Societa Editoriale Farmaceutica.

AB Moving from the interest as immunomodulatory agent of ST789 was studied the synthesis of series of N9-alkylated hypoxanthine and adenine. The synthesis and the chem. phys. properties of these derivs. are here described.

L26 ANSWER 5 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 326797-58-4 REGISTRY
CN 9H-Purine-9-pentanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
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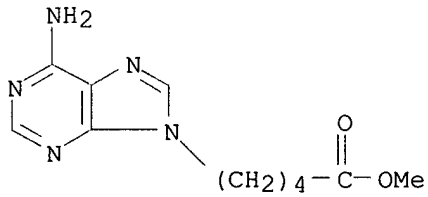
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER



Searched by: Mary Hale 308-4258 CM-1 12D16

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:178789 Synthesis of purine derivatives of potential immunomodulatory activity. Pini, E.; Rossi, E.; Ferraris, P. Cornaglia; Stradi, R. (Instituto di Chimica Organica-Facolta di Farmacia-Universita degli Studi di Milano, Milan, 20133, Italy). Bollettino Chimico Farmaceutico, 139(3), 107-113 (English) 2000. CODEN: BCFAAI. ISSN: 0006-6648. Publisher: Societa Editoriale Farmaceutica.

AB Moving from the interest as immunomodulatory agent of ST789 was studied the synthesis of series of N9-alkylated hypoxanthine and adenine. The synthesis and the chem. phys. properties of these derivs. are here described.

L26 ANSWER 6 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 223409-15-2 REGISTRY
CN 9H-Purine-9-propanoic acid, 6-amino-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
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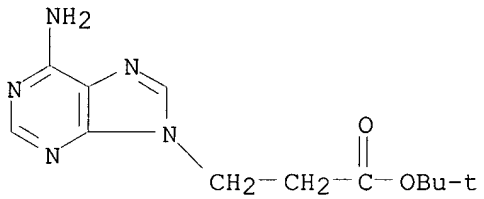
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:296947 Synthesis of acyclic carba-nucleoside phosphonates, structural analogs to natural deoxyribonucleotides. Esposito, Annamaria; Perino, Maria Grazia; Taddei, Maurizio (Dipartimento Chimica, Universita Sassari, Sassari, I-07100, Italy). Eur. J. Org. Chem. (4), 931-936 (English) 1999. CODEN: EJOCFK. ISSN: 1434-193X. Publisher: Wiley-VCH Verlag GmbH.

AB Acyclic carba-nucleoside phosphonates, modeled on natural deoxyribonucleotides were prepd. starting from DNA nucleobases and tert-Bu acrylate. The products obtained from a Michael-type reaction were elongated to .beta.-oxo esters that were first reduced to .beta.-hydroxy esters and then transformed into protected .beta.-hydroxy aldehydes. Wittig-Horner-Emmons reaction with the anion of CH2[PO(OCHMe2)2]2 gave, after deprotection, the desired 4-hydroxy-6-purinyl- or -6-pyrimidinyl-1-hexenylphosphonates. A dimer, potential precursor of acyclic polynucleotides (APN), homomorphous with DNA, was also prepd.

L26 ANSWER 7 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 194225-62-2 REGISTRY
CN 9H-Purine-9-hexanoic acid, 6-(dimethylamino)-, 5-[6-(dimethylamino)-9H-purin-9-yl]pentyl ester (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

FS 3D CONCORD
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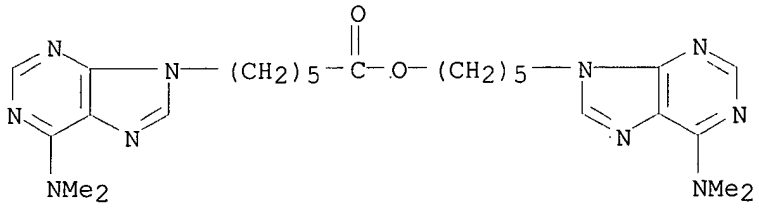
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

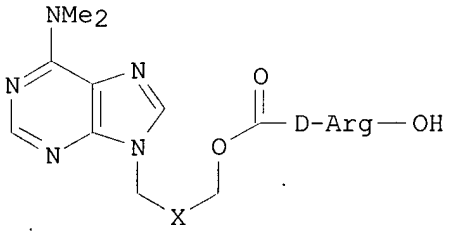


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:191025 Synthesis and Activity of 6-Substituted Purine Linker Amino Acid Immunostimulants. Zacharie, Boulos; Gagnon, Lyne; Attardo, Giorgio; Connolly, Timothy P.; St-Denis, Yves; Penney, Christopher L. (Department of Medicinal Chemistry, BioChem Therapeutic Inc., Laval, PQ, H7V 4A7, Can.). J. Med. Chem., 40(18), 2883-2894 (English) 1997. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

GI



I

AB A series of 6-substituted purinyl alkoxycarbonyl amino acids, e.g. I (X = divalent linker group) were synthesized and evaluated for their ability to stimulate cytotoxic T lymphocytes (CTLs) and the mixed lymphocyte reaction (MLR). A few of these compds., in particular I [X = (CH2)3] (BCH-1393), displayed an in vitro stimulation of CTLs comparable to interleukin 2 (IL 2). BCH-1393 increased the CTL response between 10-9 M and 10-5 M. Further, this potent in vitro activity was reflected as a significant increase in CTL cell no. in vivo. However, immunophenotyping of some of the other equipotent compds. did not reveal a parallel relative increase in CTLs in vivo. It was difficult to formulate a rigorous structure-activity relationship based on in vitro CTL activity. Nevertheless, the activity was dependent upon the nature of the 6-substituent on the purine, the type and stereochem. of the amino acid, and the distance and spatial freedom between the purine and amino acid as defined by the length and rigidity of the linker. These compds. were generally nontoxic, as exemplified by BCH-1393. BCH-1393 is a promising immunostimulant which may be targeted for those disease states which require an increased CTL or TH1 type response.

L26 ANSWER 8 OF 29 REGISTRY COPYRIGHT 2002 ACS

Searched by: Mary Hale 308-4258 CM-1 12D16

RN 188524-32-5 REGISTRY
CN 9H-Purine-9-propanoic acid, 6-amino-, octadecyl ester (9CI) (CA INDEX NAME)
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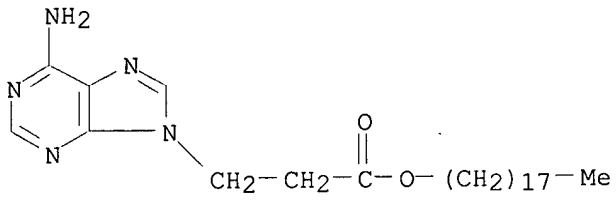
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:2125 FT-SERS Studies on Molecular Recognition Capabilities of Monolayers of Novel Nucleolipid Amphiphiles. Huang, Jianguo; Li, Chun; Liang, Yingqiu (State Key Laboratory of Coordination Chemistry and Institute of Mesoscopic Solid State Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China). Langmuir, 16(8), 3937-3940 (English) 2000. CODEN: LANGD5. ISSN: 0743-7463. Publisher: American Chemical Society.

AB The mol. recognition effect in nucleic acids was simulated in the monolayers formed by six novel nucleolipid amphiphiles. Fourier transform surface-enhanced Raman scattering (FT-SERS) technique was introduced into the research area of mol. recognition occurring in an interface system. High-quality FT-SERS spectra of a single Langmuir-Blodgett (LB) monolayer of the nucleolipid amphiphiles were obtained. Characteristic vibrational modes of the corresponding complementary nucleic acid bases, which transferred along with the monolayers of nucleolipid amphiphiles into the LB films, were clearly seen. The mechanism of mol. recognition through multiple hydrogen bonds between complementary bases was described. It was proved that this technique can be used as a powerful tool for studying mol. recognition in interface systems because of its high sensitivity.

REFERENCE 2: 129:250502 Molecular recognition of nucleolipid amphiphile octadecanoyl ester of 1-(2-carboxyethyl) adenine to the complementary nucleobases. Part I: characterization of the monolayer behavior at the air/water interface and photodimerization in the Langmuir-Blodgett film matrix under ultraviolet irradiation. Huang, Jianguo; Liang, Yingqiu (State Key Laboratory of Coordination Chemistry, Department of Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China). Thin Solid Films, 326(1,2), 217-222 (English) 1998. CODEN: THSFAP. ISSN: 0040-6090. Publisher: Elsevier Science S.A..

AB Mol. recognition capabilities of a novel nucleolipid amphiphile, octadecanoyl ester of 1-(2 carboxyethyl) adenine, to the complementary nucleobases at the air/water interface were investigated by surface pressure-area (.pi.-A) isotherms and UV spectra measurements. All of the observations show that mol. recognition through complementary base pairing takes place at the air/water interface between the adenine moiety in the headgroup of the nucleolipid amphiphile and the dissolved complementary nucleobase substrates in the subphase. On the surface of pure water, the monolayer gave a limiting mol. area of 29.3 .ANG.2 and collapse pressure

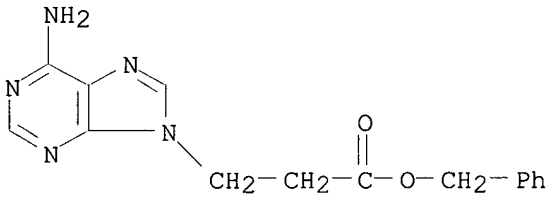
Searched by: Mary Hale 308-4258 CM-1 12D16

at .apprxeq.62 mN/m while on the subphase of aq. 5 mM thymidine and uridine soln., the limiting mol. area and collapse pressure are 42.0 .ANG.2 and 77 mN/m, 39.7 .ANG.2 and 79 mN/m, resp. In the Langmuir-Blodgett (LB) matrix, the constituent mols. are arranged regularly, which facilitates the photodimerization of the thymine moieties and uracil moieties that transferred into solid substrates along with the surface monolayer of the nucleolipid amphiphile as a result of the formation of the base-base complex, the photodimerization accomplished in 6 and 4 h for the thymine and uracil rings in the LB films under irradn. of a 254-nm UV light at room temp., resp.

REFERENCE 3: 126:238595 Synthesis of novel nucleolipid amphiphiles. Huang, Jianguo; Ding, Daoyuan; Zhang, Zhiqiang; Shi, Bo; Liang, Yingqiu (Dep. Chem., Coordination Chem. Inst. and State Key Lab. Coordination Chem., Nanjing Univ., Nanjing, 210093, Peop. Rep. China). Synth. Commun., 27(4), 681-690 (English) 1997. CODEN: SYNCAV. ISSN: 0039-7911. Publisher: Dekker.

AB Three derivs. of uridine, thymidine and adenosine with one or two stearoyl chains, and three kinds of lipids with one or two nucleic acid bases were synthesized, which can form a stable monolayer at the air-water interface.

L26 ANSWER 9 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 183181-59-1 REGISTRY
CN 9H-Purine-9-propanoic acid, 6-amino-, phenylmethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H15 N5 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

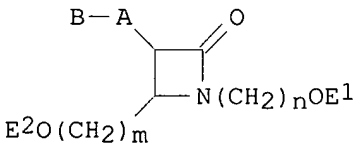


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:329293 Preparation of .beta.-lactam nucleic acids. Ravikumar, Vasulinga; Mohan, Venkatraman (Isis Pharmaceuticals, Inc., USA). U.S. US 5554746 A 19960910, 18 pp. (English). CODEN: USXXAM. APPLICATION: US 1994-243368 19940516.

GI



I

AB .beta.-Lactam monomers [I; A = [C(R6)R7]x; R6, R7 = H, alkyl, aryl, alkyl

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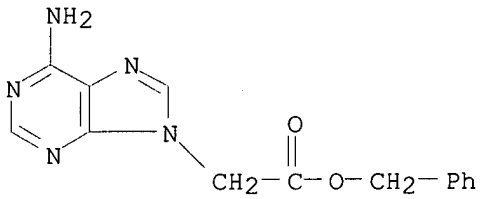
(un)substituted NH2, etc.; x = 0-10; B = adenine, guanine, thymine, cytosine, uracil; E1, E2 = H, OH-protecting group; m, n = 0-6], which can be joined into oligomeric compds. such as via preferred phosphate linkages including phosphodiester and phosphorothioate linkages, which are useful as diagnostic and research reagents (no data), are prepd.

L26 ANSWER 10 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 183181-27-3 REGISTRY
CN 9H-Purine-9-acetic acid, 6-amino-, phenylmethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H13 N5 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

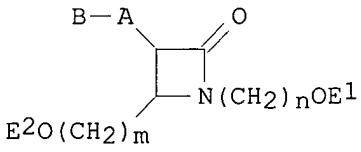


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:329293 Preparation of .beta.-lactam nucleic acids. Ravikumar, Vasulinga; Mohan, Venkatraman (Isis Pharmaceuticals, Inc., USA). U.S. US 5554746 A 19960910, 18 pp. (English). CODEN: USXXAM. APPLICATION: US 1994-243368 19940516.

GI



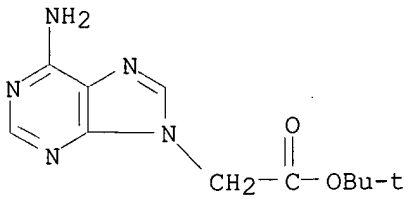
I

AB .beta.-Lactam monomers [I; A = [C(R6)R7]x; R6, R7 = H, alkyl, aryl, alkyl (un)substituted NH2, etc.; x = 0-10; B = adenine, guanine, thymine, cytosine, uracil; E1, E2 = H, OH-protecting group; m, n = 0-6], which can be joined into oligomeric compds. such as via preferred phosphate linkages including phosphodiester and phosphorothioate linkages, which are useful as diagnostic and research reagents (no data), are prepd.

L26 ANSWER 11 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 152774-16-8 REGISTRY
CN 9H-Purine-9-acetic acid, 6-amino-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
OTHER NAMES:
CN N9-[(tert-Butoxycarbonyl)methyl]adenine
FS 3D CONCORD
MF C11 H15 N5 O2
SR CA

Searched by: Mary Hale 308-4258 CM-1 12D16

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

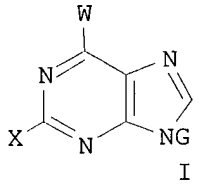


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:95606 Procedure for the production of substituted purine derivatives, the agents containing them and their use as medicaments. Peyman, Anuschirwan; Knolle, Jochen; Wehner, Volkmar; Breipohl, Gerhard; Gourvest, Jean-Francois; Carniato, Denis; Gadek, Thomas Richard (Hoechst A.-G., Germany; Genentech Inc.). Ger. Offen. DE 19653646 A1 19980625, 32 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1996-19653646 19961220.

GI



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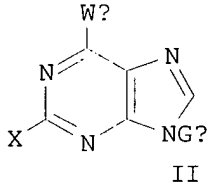
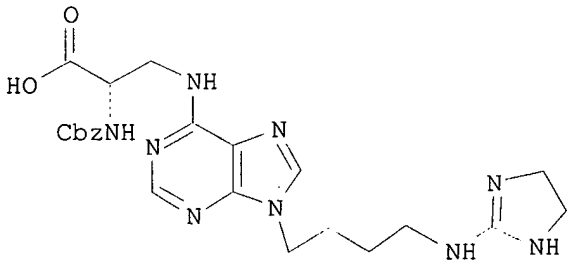


II



III

AB Purine derivs. I [G = (CR1R2)nA(CR1R2)m(CR1R3)i(CR1R2)q; W = B(CR1R2)rA1(CR1R2)s(CR1R3)k(CR1R2)tDE; X = H, NH2, NHCOR6; A, A1 = bond, CONR5, NR5CO, CO, NR5, O, S, SO, SO2, arylene, alkynylene, alkenylene; R1, R2 = H, F, Cl, CN, NO2, alkyl, cycloalkyl, (cycloalkyl)alkyl, aryl, arylalkyl, R6OR7, R6S(O)pR7, (R6)2NR7; R3 = H, F, Cl, CN, NO2, alkyl, cycloalkyl, (cycloalkyl)alkyl, aryl, arylalkyl, R6OR7, R6S(O)pR7, (R6)2NR7, R6CO2R7, R6COR7, R6OC(:O)R7, R6N(R5)CO2R7, R6S(O)pN(R5)R7, R6S(O)pN(R5)R7, R6S(O)pR7, R6SC(:O)N(R6)R7, R6COR6, R6N(R5)COR7, R6COR6, R6N(R5)COR7,R6N(R5)S(O)pR7; R4 = COR8, CSR8, S(O)pNR8, PO(R8)2, D-, L-amino acid; R5 = H, alkyl, cycloalkyl,(cycloalkyl)alkyl, aryl, arylalkyl; R6 = H, alkyl, cycloalkyl, (cycloalkyl)alkyl, aryl; R7 = bond, alkenylene; R8 = OH, alkoxy, arylalkoxy, aryloxy,

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(alkylcarbonyloxy)alkoxy, aryl(alkylcarbonyloxy)alkoxy, N(R6)2, (dialkylaminocarbonyl)methoxy, aryl(dialkylaminocarbonyl)methoxy, arylamino, L-, D-amino acid; B = O, S, NR5, NR5CO, CONR5, bond; D = bond, NR6, CONR6, NR6CO, SO2NR6, NR6CONR6, NR6CSNR6, NR6S(O)uNR6; E = H; m, n, s, t = 0 - 5; i, k = 0, 1; p, q = 0 - 2; r = 0 - 6; u = 1, 2] and. II [Ga = (CR1R2)rA1(CR1R2)s(CR1R3)k(CR1R2)tDE; Wa = B(CR1R2)nA(CR1R2)m(CR1R3)i(CR1R2)q] are useful as medicaments for treatment of osteoclastoma and retinopathy and as antiinflammation inhibitors, antitumor and cardiovascular agents. Thus, III was prepd. from 6-chloropurine via N9-alkylation with 4-MeC6H4SO3(CH2)4NHCO2CMe3, amination with H2NCH2CH(NHCbz)CO2H, and reaction with 2-(methylmercapto)-2-imidazoline hydroiodide. III showed antagonistic activity towards vitronectin receptor (.alpha..gamma..beta.3): IC50 = 0.075 .mu.M (95% inhibition at 10.mu.M).

REFERENCE 2: 128:154336 Oligonucleotide analogs with 4-hydroxy-N-acetylprolinol as sugar substitute. Ceulemans, Griet; Van Aerschot, Arthur; Wroblowski, Berthold; Rozenski, Jef; Hendrix, Chris; Herdewijn, Piet (Laboratory of Medicinal Chemistry, Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.). Chem.--Eur. J., 3(12), 1997-2010 (English) 1997. CODEN: CEUJED. ISSN: 0947-6539. Publisher: Wiley-VCH Verlag GmbH.

AB Modified oligonucleotides incorporating trans-4-hydroxy-N-acetyl-L-prolinol (trans-4-HO-L-NAP) or its D-analog as sugar substitute were synthesized with adenine and thymine as nucleobases. All-adenine oligonucleotides built from (2S,4S) or (2R,4R)-cis-4-hydroxy-N-acetylprolinol were likewise prepd. Hybridization studies revealed that hetero-complexes formed between polyU and homochiral trans-4-hydroxy-N-acetylprolinol-based oligomers of the same as well as of opposite chirality (polyU/trans-DA13* and polyU/trans-LA13*). The former, however, were triple-stranded. Other complexes with ribonucleic acids were polyA/trans-LT13* and polyU/cis-LA13*. Hetero-duplexes with deoxy-nucleic acids were formed between trans-LA13* and oligo-thymidylate. Interaction was also obsd. for cis-LA13* and oligo-thymidylate, but not with the D-hydroxyprolinol analogs. Microcalorimetry proved this interaction to be the formation of a triple-stranded complex. Two hetero-duplexes, trans-LA13*/dT13 and trans-LA13*/polyU, had similar or slightly increased stability when compared to the natural dA13/dT13 or dA13/polyU systems. Microcalorimetry clearly indicated the formation of a duplex, in contrast to interactions with N-acetylprolinol oligonucleotides of different stereochem. Moreover, the enthalpy change was of the same magnitude but the assocn. const. was slightly lower. Natural nucleic acids thus clearly prefer hybridization with L-hydroxyprolinol oligomers over D-hydroxyprolinol oligomers. For the series investigated, the L-trans oligomers seem best to mimic natural oligonucleotides. These modified oligonucleotides formed homo-complexes if both strands were of the same chirality, i.e., homo-complexes formed between trans-LA* and trans-LT* and between trans-DA* and trans-DT*, reflecting the iso-chiral pu-py pairing found in natural nucleic acids. Once more, however, calorimetry proved these to be triplex interactions. Hetero-chiral pairing was not obsd. between modified oligonucleotides, but only between modified oligonucleotides and natural polyU. The thermal stabilities of these hetero-chiral complexes differed clearly.

REFERENCE 3: 126:131753 PNA-DNA chimeras and PNA synthons for their preparation. Gildea, Brian D.; Coull, James M. (Perseptive Biosystems, Inc., USA). PCT Int. Appl. WO 9640709 A1 19961219, 99 pp. DESIGNATED STATES: W: JP; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US7844 19960529. PRIORITY: US 1995-480228 19950607.

AB A method is disclosed for the prepn. of novel peptide nucleic acid (PNA) synthons compatible with DNA synthetic reagents and instrumentation.

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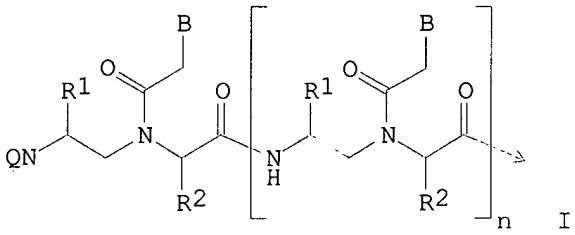
Accordingly, the PNA synthons of this invention are particularly suitable for the prepn. of PNA-DNA chimeras, among other oligomers. The PNA synthons are designed to have a protecting group strategy which is orthogonal and allows removal of the protecting groups under mild conditions. Generally, an acid labile protected backbone is coupled to a nucleobase side chain moiety to form the PNA synthon. A novel method for synthesizing the acid labile protected backbone also is described. In addn., novel compns. of matter are disclosed.

REFERENCE 4: 120:135140 Peptide nucleic acids and their effect on genetic material. Thomson, Stephen A.; Noble, Stewart A.; Ricca, Daniel J. (Glaxo Inc., USA). PCT Int. Appl. WO 9312129 A1 19930624, 49 pp. DESIGNATED STATES: W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, UA, US; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1992-US10921 19921217. PRIORITY: US 1991-809661 19911218.

GI



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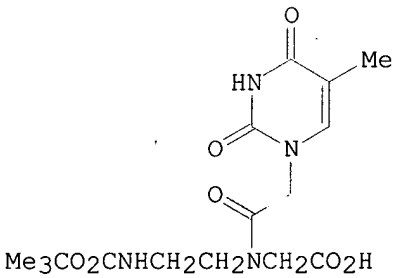
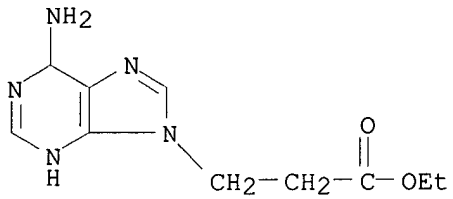


III

AB Nucleic acid base-contg. peptides I [B = nucleic acid base; Q, J = protective group; QJ = bond; R1, R2 = H, (un)substituted alkyl, aryl, heteroaryl; n= .gtoreq.1] were prepd. for use as inhibitors of genetic transcription. Thus, I [Q, R1, R2 = H, J = NH2, B = thymine; n = 5, II] was prepd. from resin-bound lysine and the monomer III which was obtained by reductive alkylation of H2NCH2CO2Me.HCl with Me3CO2CNHCH2CHO, followed by reaction with 1-carboxymethylthymine. II inhibited poly rA.T25-30 duplex formation at .gtoreq.0.1 .mu.M.

L26 ANSWER 12 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 138137-08-3 REGISTRY
CN 9H-Purine-9-propanoic acid, 6-amino-1,6-dihydro-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H15 N5 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Searched by: Mary Hale 308-4258 CM-1 12D16

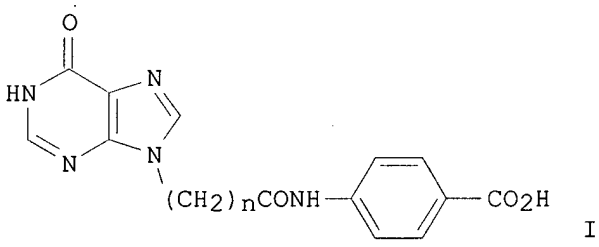


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:366899 Preparation and use of 9-substituted hypoxanthines to stimulate regeneration of mammalian motor neurons.. Glasky, Alvin (Neotherapeutics, Inc., USA). PCT Int. Appl. WO 2001036419 A1 20010525, 26 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US41645 20001027. PRIORITY: US 1999-442151 19991116.

GI



I

AB A method of stimulating regeneration or survival of a mammalian motor neuron comprises administration of title compds. (I; n = 1-6). Preferably, the compd. is N-4-carboxyphenyl 3-(6-oxohydropurin-9-yl) propanamide (II). Thus, adenine in EtOH was treated with Na and then with H2C:CHCO2Et followed by 18 h reflux to give 87% Et 3-(1,6-dihydro-6-amino-9H-purin-9-yl)propionate. The latter in HOAc was treated with aq. NaNO2 followed by stirring for 24 h to give 30% Et 3-(1,6-dihydro-6-oxo-9H-purin-9-yl)propionate. This was converted to II in 4 steps. II in rats with spinal cord lesions increased levels of mRNA for neurotrophic factors at the lesion site.

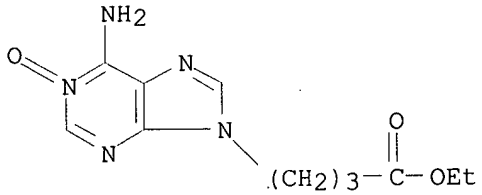
REFERENCE 2: 116:15822 Multifunctional pharmaceutical compounds and methods of use. Glasky, Alvin J. (USA). PCT Int. Appl. WO 9114434 A1 19911003, 65 pp. DESIGNATED STATES: W: AU, BR, CA, FI, HU, JP, KR, MC, NO, SU; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1991-US2066 19910326. PRIORITY: US 1990-500789 19900328.

AB Multifunctional pharmaceuticals comprise .gtoreq.2 biol. active chem. groups linked by a chem. bridging group. The compds. are useful for treating degenerative diseases and interrelated physiol. systems.

Searched by: Mary Hale 308-4258 CM-1 12D16

3-(1,6-Dihydro-6-oxo-9H-purin-9-yl)propanoic acid (AIT-0080) enhanced T-lymphocyte proliferation at a moderate dosage (10 .mu.g/mL), yet enhanced B-lymphocyte function at relatively low dosage (1 .mu.g/mL). Addnl., AIT-0080 enhanced memory function as well as locomotor activity at 0.5 mg/kg in vivo. AIT-0080 was prepd. from adenine in 3 steps.

L26 ANSWER 13 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 130080-69-2 REGISTRY
CN 9H-Purine-9-butanoic acid, 6-amino-, ethyl ester, 1-oxide (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H15 N5 O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

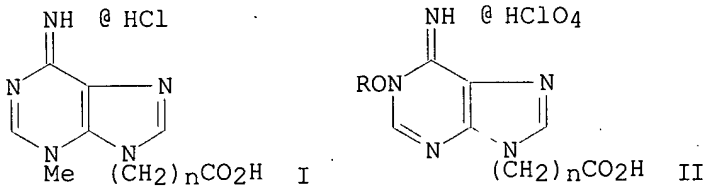


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:191038 Purines. XL. Preparation of 9-(.omega.-carboxyalkyl)-3-methyladenines. Fujii, Tozo; Saito, Tohru; Kumazawa, Yukinari (Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan). Chem. Pharm. Bull., 38(5), 1392-5 (English) 1990. CODEN: CPBTAL. ISSN: 0009-2363.

GI

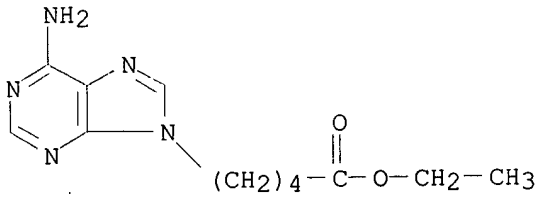


AB With a view to supplying haptens to be connected to carrier proteins for raising antibodies to 3-methyl-2'-deoxyadenosine and/or 3-methyladenine, the title compds. I (n = 1, 3) have been prepd. from 1-alkoxy-9-(.omega.-carboxyalkyl)adenine salts II (n = 1, R = Et; n = 3, R = Me).

L26 ANSWER 14 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 102788-98-7 REGISTRY
CN 9H-Purine-9-pentanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H17 N5 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

Searched by: Mary Hale 308-4258 CM-1 12D16

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:238179 Polymethylene derivatives of nucleic bases with .omega.-functional groups: II. Adenine and hypoxanthine derivatives. Makinsky, A. A.; Kritzyn, A. M.; Ul'yanova, E. A.; Zakharova, O. D.; Bugreev, D. V.; Nevinsky, G. A. (Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, 119991, Russia). Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya), 27(3), 167-172 (English) 2001. CODEN: RJBCET. ISSN: 1068-1620. Publisher: MAIK Nauka/Interperiodica.

AB N9-Polymethylene derivs. of adenine and hypoxanthine with various functional groups in the .omega.-position of the alkyl substituent were synthesized. Their physicochem. properties and effect on the HIV reverse transcriptase and DNA topoisomerase I were studied.

REFERENCE 2: 126:7881 Synthesis and some spectroscopic properties of porphyrin derivatives connected with nucleobases (adenine, thymine, guanine and cytosine) by alkanamide chains. Hisatome, Masao; Maruyama, Noriaki; Ikeda, Koichi; Furutera, Tetsuo; Ishikawa, Tomiyasu; Yamakawa, Koji (Fac. Pharmaceutical Sciences, Science Univ. Tokyo, Tokyo, 162, Japan). Chem. Pharm. Bull., 44(10), 1801-1811 (English) 1996. CODEN: CPBTAL. ISSN: 0009-2363. Publisher: Pharmaceutical Society of Japan.

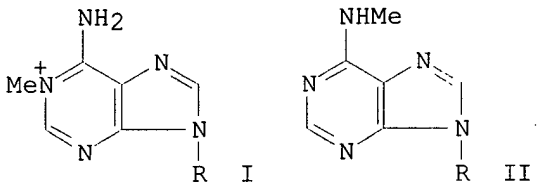
AB Several kinds of porphyrin derivs. covalently connected with adenine, thymine, guanine, cytosine or with the adenine-thymine pair in a stacking mode have been synthesized via amidation of (2-aminophenyl)porphyrin derivs. with nucleobase-alkanoic acids, and characterized by spectroscopic methods. In the 1H-NMR spectra of these nucleobase-porphyrins the proton signals of the nucleobase moieties appear at remarkably higher fields than those of the ref. compds. (the corresponding nucleobase-alkanoates) which have no porphyrin moiety. The behaviors of the high field shifts, due to the diamagnetic ring current effect of the porphyrin ring, reflect the characteristic conformational features of these compds. in which the base moieties are located at the upper zone of the porphyrin ring. The Soret bands of the porphyrin in the electronic absorption spectra were markedly weaker in intensity compared with those of the ref. compd. which has no nucleobase moiety. Both the high-field shifts of the base protons and the hypochromic effects on the Soret band are larger in guanine and cytosine systems than those in adenine and thymine systems, resp. These results indicate a greater affinity of guanine and cytosine for porphyrin in comparison with adenine and cytosine, resp., and this conclusion is compatible with the reported electronic spectral properties of mixts. of polynucleotides and water-sol. porphyrin derivs.

REFERENCE 3: 105:24556 Purines. XXVI. The Dimroth rearrangement of 9-substituted 1-methyladenines: accelerating effect of a .beta.-D-ribofuranosyl group at the 9-position. Fujii, Tozo; Saito, Tohru

Searched by: Mary Hale 308-4258 CM-1 12D16

(Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan). Chem. Pharm. Bull., 33(9), 3635-44 (English) 1985. CODEN: CPBTAL. ISSN: 0009-2363.

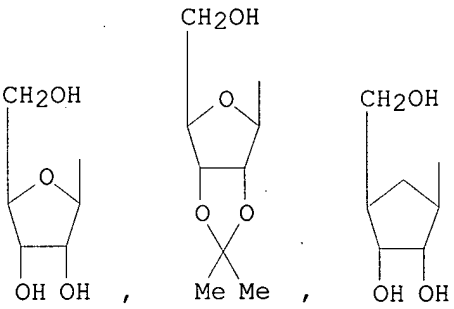
GI



I

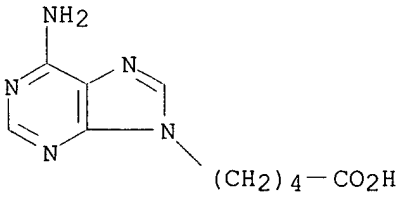
II

R1=



AB The reaction rates in the Dimroth rearrangements of 1-methyladenines I [R = Me, Et, CH2Ph2 (CH2)4OH, (CH2)5OH, R1] to purines II were measured in H2O at various pH's and ionic strength 1.0 and 40 .degree.C. In all cases, attack of hydroxide ion on the protonated species of I at the 2-position was faster than that on the neutral species by a factor of 90-180. I (R = .beta.-D-ribofuranosyl) was found to accelerate both modes of hydroxide attack most significantly. This rate enhancement is attributable solely to the electron-withdrawing effect of the furanose ring oxygen and not to the 5'-hydroxy group, a potential participant in intramol. catalysis for the hydroxide attack on the adenine ring at the 2-position.

L26 ANSWER 15 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 90973-36-7 REGISTRY
CN 9H-Purine-9-pentanoic acid, 6-amino- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 9H-Purine-9-valeric acid, 6-amino- (7CI)
FS 3D CONCORD
MF C10 H13 N5 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 12D16

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 135:238179 Polymethylene derivatives of nucleic bases with .omega.-functional groups: II. Adenine and hypoxanthine derivatives. Makinsky, A. A.; Kritzyn, A. M.; Ul'yanova, E. A.; Zakharova, O. D.; Bugreev, D. V.; Nevinsky, G. A. (Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, 119991, Russia). Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya), 27(3), 167-172 (English) 2001. CODEN: RJBCET. ISSN: 1068-1620. Publisher: MAIK Nauka/Interperiodica.

AB N9-Polymethylene derivs. of adenine and hypoxanthine with various functional groups in the .omega.-position of the alkyl substituent were synthesized. Their physicochem. properties and effect on the HIV reverse transcriptase and DNA topoisomerase I were studied.

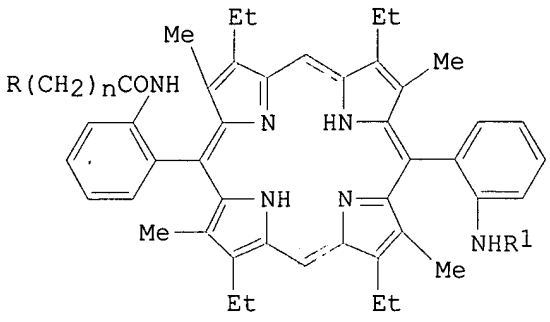
REFERENCE 2: 126:7881 Synthesis and some spectroscopic properties of porphyrin derivatives connected with nucleobases (adenine, thymine, guanine and cytosine) by alkanamide chains. Hisatome, Masao; Maruyama, Noriaki; Ikeda, Koichi; Furutera, Tetsuo; Ishikawa, Tomiyasu; Yamakawa, Koji (Fac. Pharmaceutical Sciences, Science Univ. Tokyo, Tokyo, 162, Japan). Chem. Pharm. Bull., 44(10), 1801-1811 (English) 1996. CODEN: CPBTAL. ISSN: 0009-2363. Publisher: Pharmaceutical Society of Japan.

AB Several kinds of porphyrin derivs. covalently connected with adenine, thymine, guanine, cytosine or with the adenine-thymine pair in a stacking mode have been synthesized via amidation of (2-aminophenyl)porphyrin derivs. with nucleobase-alkanoic acids, and characterized by spectroscopic methods. In the 1H-NMR spectra of these nucleobase-porphyrins the proton signals of the nucleobase moieties appear at remarkably higher fields than those of the ref. compds. (the corresponding nucleobase-alkanoates) which have no porphyrin moiety. The behaviors of the high field shifts, due to the diamagnetic ring current effect of the porphyrin ring, reflect the characteristic conformational features of these compds. in which the base moieties are located at the upper zone of the porphyrin ring. The Soret bands of the porphyrin in the electronic absorption spectra were markedly weaker in intensity compared with those of the ref. compd. which has no nucleobase moiety. Both the high-field shifts of the base protons and the hypochromic effects on the Soret band are larger in guanine and cytosine systems than those in adenine and thymine systems, resp. These results indicate a greater affinity of guanine and cytosine for porphyrin in comparison with adenine and cytosine, resp., and this conclusion is compatible with the reported electronic spectral properties of mixts. of polynucleotides and water-sol. porphyrin derivs.

REFERENCE 3: 114:101481 Porphyrins coupled with nucleoside bases. Synthesis and characterization of adenine- and thymine-porphyrin derivatives. Hisatome, Masao; Maruyama, Noriaki; Furutera, Tetsuo; Ishikawa, Tomoyasu; Yamakawa, Koji (Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan). Chem. Lett. (12), 2251-4 (English) 1990. CODEN: CMLTAG. ISSN: 0366-7022.

GI

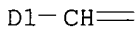
Searched by: Mary Hale 308-4258 CM-1 12D16

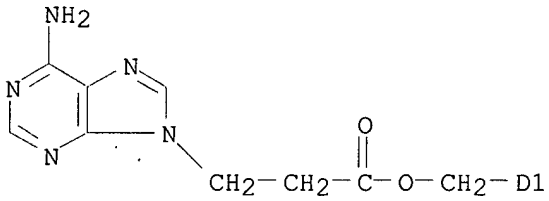


I

AB Porphyrins I (R = adenyl, thyminyl; R1 = H, CO2Et, CO2CH2Ph; n = 3, 4) have been synthesized. Spectroscopic study suggested an interaction between the porphyrin ring and the base moiety, and indicated nucleoside base recognition ability of the compds.

L26 ANSWER 16 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 83372-27-4 REGISTRY
CN 9H-Purine-9-propanoic acid, 6-amino-, (ethenylphenyl)methyl ester (9CI) (CA INDEX NAME)
MF C17 H17 N5 O2
CI IDS, COM
LC STN Files: CA, CAPLUS





1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 97:163584 Spacer effect in the template polycondensation of nucleotide analogs with diamines. Nakagawa, Hiroshi; Muraki, Michiro; Miura, Yozo; Kinoshita, Masayoshi (Fac. Eng., Osaka City Univ., Osaka, Japan). Makromol. Chem., 183(9), 2065-70 (English) 1982. CODEN: MACEAK. ISSN: 0025-116X.

AB The template effect of polystyrene contg. 3-(9-adenylpropionyl)oxymethyl group bounded via a styrene spacer group. on the polycondensation of active esters [bis(p-nitrophenyl) 2-(thymin-1-ylmethyl)succinate (I) and bis(2-nitrophenyl) 2-(theophyllin-7-ylmethyl)succinate (II)] with diamines was studied in pyridine-CH2Cl2 or DMF. Template polymers accelerated the polycondensation of I with diamines by a factor of 5-20, but the

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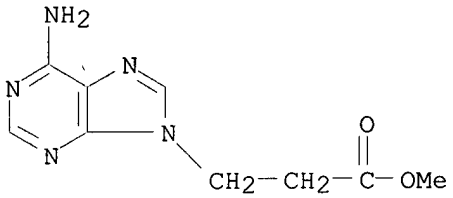
polycondensation of II with piperazine showed no appreciable template effect.

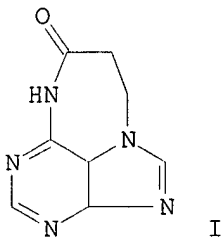
L26 ANSWER 17 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 70259-15-3 REGISTRY
CN 9H-Purine-9-propanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H11 N5 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 102:220644 Some intramolecular Michael additions of adenine derivatives. Brahme, Nanda M.; Smith, Walter T., Jr. (Dep. Chem., Univ. Kentucky, Lexington, KY, 45006-0055, USA). J. Heterocycl. Chem., 22(1), 109-12 (English) 1985. CODEN: JHTCAD. ISSN: 0022-152X.
GI



I

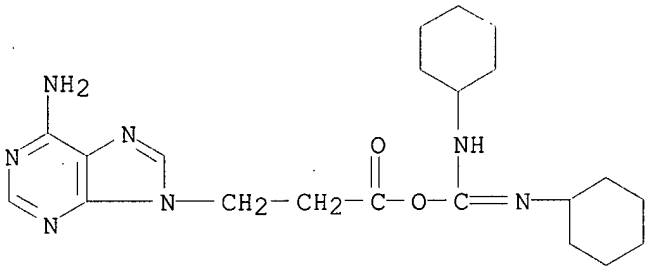
AB Reaction of adenine with acrylic anhydride or vinyl acrylate in Me2SO was accompanied by intramol. Michael addn. to give the diazepinopurine I which was hydrolyzed with 1N NaOH to give 7-carboxyethyladenine. Reaction of adenine with various acrylic derivs. in DMF or aq. NaOH gave 3-carboxyethyladenine. Adenine reacted with CH2:CHCN or Me acrylate in Me2SO to give a mixt. of the 7- and 9-substituted derivs.

REFERENCE 2: 91:20943 Synthesis of new mono- and disubstituted hydroxyalkyl and aminoalkyl derivatives of heterocyclic bases. Holy, Antonin (Inst. Org. Chem. Biochem., Czechoslovak Acad. Sci., Prague, Czech.). Collect. Czech. Chem. Commun., 43(12), 3444-65 (English) 1978. CODEN: CCCCAK. ISSN: 0366-547X.
AB Adenine derivs. contg. an aliph. chain with 1 or 2 OH, NH2, or OMe groups and also some derivs. of the corresponding carboxylic acids were prepd.

Searched by: Mary Hale 308-4258 CM-1 12D16

Several analogs contg. other heterocycles were also prepd. The compds. were prepd. for screening for antibacterial and antiviral activities; none of the compds. were inhibitory against Escherichia coli at concns. up to 1000 .mu.g/mL (results of antiviral screening not given). Thus, reaction of adenine with Me acrylate gave 3-(adenin-9-yl)- (I) and 3-(adenin-3-yl)propionic acid. Esterification of I with CH2N2 and redn. of the ester with NaBH4 gave 9-(3-hydroxypropyl)adenine.

L26 ANSWER 18 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 57992-44-6 REGISTRY
CN 9H-Purine-9-propanoic acid, 6-amino-, anhydride with N,N'-dicyclohexylcarbamimidic acid (9CI) (CA INDEX NAME)
MF C21 H31 N7 O2
LC STN Files: CA, CAPLUS



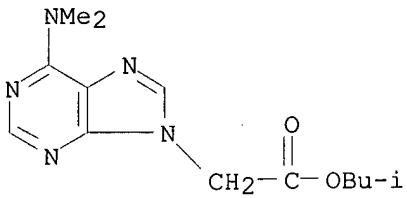
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 84:60038 Functional monomers and polymers. 28. Synthesis and polymerization of nucleic-base containing styrene derivatives. Kondo, Koichi; Sato, Toshiaki; Inaki, Yoshiaki; Takemoto, Kiichi (Tech. Fac., Univ. Osaka, Suita, Japan). Makromol. Chem., 176(11), 3505-9 (German) 1975. CODEN: MACEAK.
GI For diagram(s), see printed CA Issue.
AB The reaction of uracil [66-22-8], thymine [65-71-4], or theophylline [58-55-9] with propiolactone (I) [57-57-8] and 4-aminostyrene (II) [1520-21-4] gave compound III [57992-45-7] and analogous thymine and theophylline derivs. which were homopolymd. or copolymd. with styrene in the presence of AIBN. The reaction of adenine [73-24-5] with I and II gave 9-[3-oxo-3-(4-vinylanilino)-1-propyl]adenine polymer [57998-20-6].

L26 ANSWER 19 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 55175-42-3 REGISTRY
CN 9H-Purine-9-acetic acid, 6-(dimethylamino)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H19 N5 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

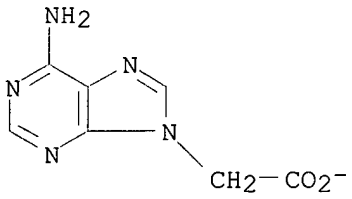
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 82:140427 Oxidation of reversed nucleosides in oxygen. III. Synthesis of eritadenine analogs of purines and pyrimidines. Kanno, Takeshi; Kawazu, Mitsutaka (Org. Chem. Res. Lab., Tanabe Seiyaku Co., Ltd., Toda, Japan). Chem. Pharm. Bull., 22(12), 2836-50 (English) 1974. CODEN: CPBTAL.

GI For diagram(s), see printed CA Issue.

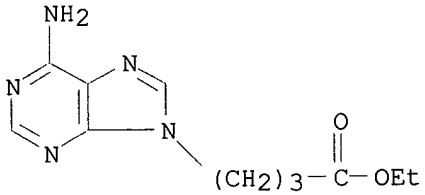
AB Reaction of Me 5-O-tosyl-2,3-O-isopropylidene-.beta.-D-ribofuranoside with the Na salts of purines and pyrimidines in DMF afforded the corresponding reversed nucleosides. 6-Alkylaminopurine analogs I (R = NHBu, NMe2, furfurylamino) were prepd. by the reaction of I (R = SMe) with amines. After deblocking, the reversed nucleosides were oxidized by O in dil. alk. soln. to afford eritadenine analogs.

L26 ANSWER 20 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 49859-53-2 REGISTRY
CN 9H-Purine-9-acetic acid, 6-amino-, ion(1-) (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C7 H6 N5 O2
CI COM



L26 ANSWER 21 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 41785-06-2 REGISTRY
CN 9H-Purine-9-butanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Ethyl 4-(adenin-9-yl)butyrate
FS 3D CONCORD
MF C11 H15 N5 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1967 TO DATE)
5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

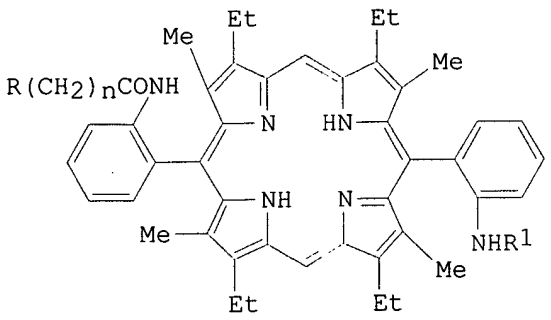
REFERENCE 1: 126:7881 Synthesis and some spectroscopic properties of porphyrin derivatives connected with nucleobases (adenine, thymine, guanine and cytosine) by alkanamide chains. Hisatome, Masao; Maruyama, Noriaki; Ikeda, Koichi; Furutera, Tetsuo; Ishikawa, Tomiyasu; Yamakawa, Koji (Fac. Pharmaceutical Sciences, Science Univ. Tokyo, Tokyo, 162, Japan). Chem. Pharm. Bull., 44(10), 1801-1811 (English) 1996. CODEN: CPBTAL. ISSN: 0009-2363. Publisher: Pharmaceutical Society of Japan.

AB Several kinds of porphyrin derivs. covalently connected with adenine, thymine, guanine, cytosine or with the adenine-thymine pair in a stacking mode have been synthesized via amidation of (2-aminophenyl)porphyrin derivs. with nucleobase-alkanoic acids, and characterized by spectroscopic methods. In the 1H-NMR spectra of these nucleobase-porphyrins the proton signals of the nucleobase moieties appear at remarkably higher fields than those of the ref. compds. (the corresponding nucleobase-alkanoates) which have no porphyrin moiety. The behaviors of the high field shifts, due to the diamagnetic ring current effect of the porphyrin ring, reflect the characteristic conformational features of these compds. in which the base moieties are located at the upper zone of the porphyrin ring. The Soret bands of the porphyrin in the electronic absorption spectra were markedly weaker in intensity compared with those of the ref. compd. which has no nucleobase moiety. Both the high-field shifts of the base protons and the hypochromic effects on the Soret band are larger in guanine and cytosine systems than those in adenine and thymine systems, resp. These results indicate a greater affinity of guanine and cytosine for porphyrin in comparison with adenine and cytosine, resp., and this conclusion is compatible with the reported electronic spectral properties of mixts. of polynucleotides and water-sol. porphyrin derivs.

REFERENCE 2: 114:101481 Porphyrins coupled with nucleoside bases. Synthesis and characterization of adenine- and thymine-porphyrin derivatives. Hisatome, Masao; Maruyama, Noriaki; Furutera, Tetsuo; Ishikawa, Tomoyasu; Yamakawa, Koji (Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan). Chem. Lett. (12), 2251-4 (English) 1990. CODEN: CMLTAG. ISSN: 0366-7022.

GI

Searched by: Mary Hale 308-4258 CM-1 12D16

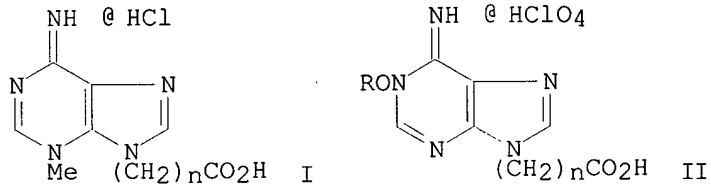


I

AB Porphyrins I (R = adenyl, thyminyl; R1 = H, CO2Et, CO2CH2Ph; n = 3, 4) have been synthesized. Spectroscopic study suggested an interaction between the porphyrin ring and the base moiety, and indicated nucleoside base recognition ability of the compds.

REFERENCE 3: 113:191038 Purines. XL. Preparation of 9-(.omega.-carboxyalkyl)-3-methyladenines. Fujii, Tozo; Saito, Tohru; Kumazawa, Yukinari (Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan). Chem. Pharm. Bull., 38(5), 1392-5 (English) 1990. CODEN: CPBTAL. ISSN: 0009-2363.

GI



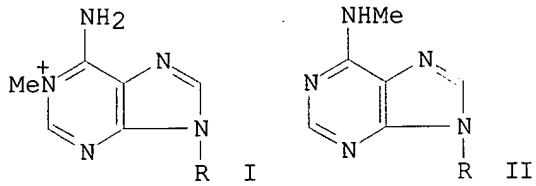
I II

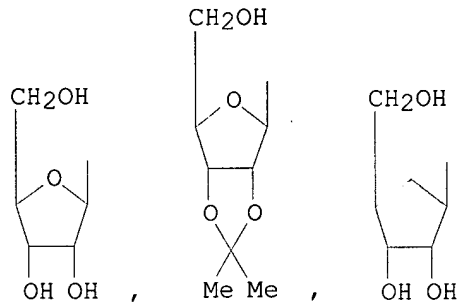
AB With a view to supplying haptens to be connected to carrier proteins for raising antibodies to 3-methyl-2'-deoxyadenosine and/or 3-methyladenine, the title compds. I (n = 1, 3) have been prepd. from 1-alkoxy-9-(.omega.-carboxyalkyl)adenine salts II (n = 1, R = Et; n = 3, R = Me).

REFERENCE 4: 105:24556 Purines. XXVI. The Dimroth rearrangement of 9-substituted 1-methyladenines: accelerating effect of a .beta.-D-ribofuranosyl group at the 9-position. Fujii, Tozo; Saito, Tohru (Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan). Chem. Pharm. Bull., 33(9), 3635-44 (English) 1985. CODEN: CPBTAL. ISSN: 0009-2363.

GI

Searched by: Mary Hale 308-4258 CM-1 12D16



R1= 

AB The reaction rates in the Dimroth rearrangements of 1-methyladenines I [R = Me, Et, CH2Ph2 (CH2)4OH, (CH2)5OH, R1] to purines II were measured in H2O at various pH's and ionic strength 1.0 and 40 .degree.C. In all cases, attack of hydroxide ion on the protonated species of I at the 2-position was faster than that on the neutral species by a factor of 90-180. I (R = .beta.-D-ribofuranosyl) was found to accelerate both modes of hydroxide attack most significantly. This rate enhancement is attributable solely to the electron-withdrawing effect of the furanose ring oxygen and not to the 5'-hydroxy group, a potential participant in intramol. catalysis for the hydroxide attack on the adenine ring at the 2-position.

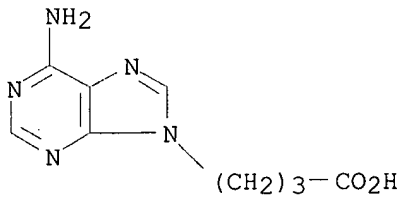
REFERENCE 5: 79:42452 Synthetic spectroscopic models related to coenzymes and base pairs. XII. Controlled interaction between nucleic acid bases. Intramolecular stacking interactions between two adenine rings. Leonard, Nelson J.; Ito, Keiichi (Sch. Chem. Sci., Univ. Illinois, Urbana, Ill., USA). J. Amer. Chem. Soc., 95(12), 4010-16 (English) 1973. CODEN: JACSAT.

AB To det. the stacking interactions between two parallel rings oriented at different axis angles toward each other, a series of six different trimethylenebisadenine isomers was synthesized. The per cent hypochromism, H, for the long wavelength uv absorption band for each of these compds was detd. by comparison of the uv spectrum of the trimethylenebisadenine in aq. soln. with the composite spectrum of the two half mol., the appropriate propyladenines. The H values obtained thereby for the trimethylenebisadenines are the following: 9,9'isomer, 15%; N6,N6', 16%; 8,8', 21%; N6,9', 16%; 8,9', 19%; 7,9', 16%. The per cent hypochromism follows a dependence upon the folded confor- mations available to the individual trimethylenebisadenines and offers the possiblity of assessing the degree and orientation of overlap per- mitted or excluded for different ranges of H values.

L26 ANSWER 22 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 33147-28-3 REGISTRY
CN 9H-Purine-9-butanoic acid, 6-amino- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 9H-Purine-9-butyric acid, 6-amino- (8CI)
OTHER NAMES:
CN 4-(Aden-9-yl)butyric acid

Searched by: Mary Hale 308-4258 CM-1 12D16

FS 3D CONCORD
MF C9 H11 N5 O2
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1967 TO DATE)
7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:7881 Synthesis and some spectroscopic properties of porphyrin derivatives connected with nucleobases (adenine, thymine, guanine and cytosine) by alkanamide chains. Hisatome, Masao; Maruyama, Noriaki; Ikeda, Koichi; Furutera, Tetsuo; Ishikawa, Tomiyasu; Yamakawa, Koji (Fac. Pharmaceutical Sciences, Science Univ. Tokyo, Tokyo, 162, Japan). Chem. Pharm. Bull., 44(10), 1801-1811 (English) 1996. CODEN: CPBTAL. ISSN: 0009-2363. Publisher: Pharmaceutical Society of Japan.

AB Several kinds of porphyrin derivs. covalently connected with adenine, thymine, guanine, cytosine or with the adenine-thymine pair in a stacking mode have been synthesized via amidation of (2-aminophenyl)porphyrin derivs. with nucleobase-alkanoic acids, and characterized by spectroscopic methods. In the 1H-NMR spectra of these nucleobase-porphyrins the proton signals of the nucleobase moieties appear at remarkably higher fields than those of the ref. compds. (the corresponding nucleobase-alkanoates) which have no porphyrin moiety. The behaviors of the high field shifts, due to the diamagnetic ring current effect of the porphyrin ring, reflect the characteristic conformational features of these compds. in which the base moieties are located at the upper zone of the porphyrin ring. The Soret bands of the porphyrin in the electronic absorption spectra were markedly weaker in intensity compared with those of the ref. compd. which has no nucleobase moiety. Both the high-field shifts of the base protons and the hypochromic effects on the Soret band are larger in guanine and cytosine systems than those in adenine and thymine systems, resp. These results indicate a greater affinity of guanine and cytosine for porphyrin in comparison with adenine and cytosine, resp., and this conclusion is compatible with the reported electronic spectral properties of mixts. of polynucleotides and water-sol. porphyrin derivs.

REFERENCE 2: 119:117014 Porphyrins coupled with nucleoside bases. Synthesis and some properties of guanine, cytosine and adenine-thymine derivatives. Hisatome, Masao; Maruyama, Noriaki; Ikeda, Koichi; Yamakawa, Koji (Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan). Heterocycles, 36(3), 441-4 (English) 1993. CODEN: HTCYAM. ISSN: 0385-5414.

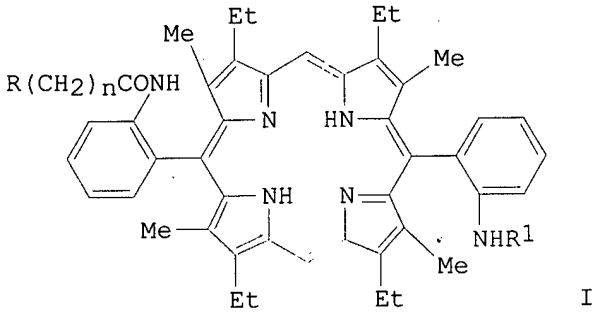
AB Synthesis of several porphyrin derivs. having a guanine, cytosine or adenine-thymine pair is described. Diamagnetic shift behaviors of the base proton signals in the 1H NMR spectra of the derivs. and hypochromism of the Soret band in the electronic spectra are briefly discussed.

REFERENCE 3: 114:101481 Porphyrins coupled with nucleoside bases. Synthesis and characterization of adenine- and thymine-porphyrin derivatives.

Searched by: Mary Hale 308-4258 CM-1 12D16

Hisatome, Masao; Maruyama, Noriaki; Furutera, Tetsuo; Ishikawa, Tomoyasu; Yamakawa, Koji (Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan). Chem. Lett. (12), 2251-4 (English) 1990. CODEN: CMLTAG. ISSN: 0366-7022.

GI



I

AB Porphyrins I (R = adenyl, thyminyl; R1 = H, CO2Et, CO2CH2Ph; n = 3, 4) have been synthesized. Spectroscopic study suggested an interaction between the porphyrin ring and the base moiety, and indicated nucleoside base recognition ability of the compds.

REFERENCE 4: 82:25663 Synthesis and hypocholesterolemic activities of eritadenine derivatives. Okumura, Kentaro; Matsumoto, Kazuo; Fukamizu, Masaharu; Yasuo, Harunori; Taguchi, Yoshihiko; Sugihara, Yukio; Inoue, Ichizo; Seto, Masahiko; Sato, Yasuhiko; et al. (Res. Lab., Tanabe Seiyaku Co., Ltd., Toda, Japan). J. Med. Chem., 17(8), 846-55 (English) 1974. CODEN: JMCMAR.

GI For diagram(s), see printed CA Issue.

AB More than 100 title compds. were prepd. by esterification or amidation of eritadenine (I) [23918-98-1], alkylation of adenine [73-24-5] with O-protected 2(R),3(R)-Et 4-bromo-2,3-dihydroxybutyrate [53186-35-9], or ring closure of appropriate aminocyanoimidazolylribonucleosides followed by hydrolysis and oxidn. In tests in rats for hypocholesterolemic activity, esters of I with short chain alcs. were 25 to 50 times as active as I, with a minimal effective dose in diet as low as 0.1 mg/kg/day. I is about 10 times as active as clofibrate [637-07-0]. Structure-activity relations were discussed.

REFERENCE 5: 82:327 Hypocholesterolemic activity of analogous compounds related to eritadenine, and active component of Shiitake, Lentinus edodes. Tensho, Akira; Shimizu, Iwao; Takenawa, Tadaomi; Kikuchi, Hiroyuki; Rokujo, Tsuneshige; Kamiya, Takashi (Res. Lab., Fujisawa Pharm. Co., Ltd., Tokyo, Japan). Yakugaku Zasshi, 94(6), 708-16 (Japanese) 1974. CODEN: YKKZAJ.

GI For diagram(s), see printed CA Issue.

AB Eritadenine (I) [23918-98-1] esters given orally to rats were 10 times as active as I itself in serum cholesterol-lowering activity. The activity required the presence of purine ring in the mols. and of NH2 or similar basic substituents at the 6 position. As to the side chain of I, the presence of butyric acid with OH at .alpha. or .beta. position induced a strong activity. The activities of 66 I derivs. were studied.

REFERENCE 6: 79:42452 Synthetic spectroscopic models related to coenzymes and base pairs. XII. Controlled interaction between nucleic acid bases. Intramolecular stacking interactions between two adenine rings. Leonard, Nelson J.; Ito, Keiichi (Sch. Chem. Sci., Univ. Illinois, Urbana, Ill., USA). J. Amer. Chem. Soc., 95(12), 4010-16 (English) 1973. CODEN: JACSAT.

Searched by: Mary Hale 308-4258 CM-1 12D16

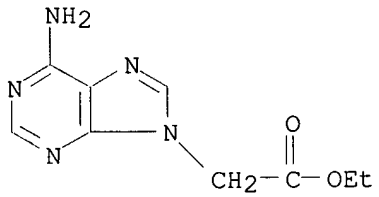
AB To det. the stacking interactions between two parallel rings oriented at different axis angles toward each other, a series of six different trimethylenebisadenine isomers was synthesized. The per cent hypochromism, H, for the long wavelength uv absorption band for each of these compds was detd. by comparison of the uv spectrum of the trimethylenebisadenine in aq. soln. with the composite spectrum of the two half mol., the appropriate propyladenines. The H values obtained thereby for the trimethylenebisadenines are the following: 9,9'isomer, 15%; N6,N6', 16%; 8,8', 21%; N6,9', 16%; 8,9', 19%; 7,9', 16%. The per cent hypochromism follows a dependence upon the folded confor- mations available to the individual trimethylenebisadenines and offers the possiblity of assessing the degree and orientation of overlap per- mitted or excluded for different ranges of H values.

REFERENCE 7: 75:63742 Novel carboxyalkylations of purines by .gamma.-lactones. De Kock, D. H.; Raubenheimer, H. G. (Dep. Chem., Univ. Stellenbosch, Stellenbosch, S. Afr.). J. S. Afr. Chem. Inst., 24(May), 91-5 (English) 1971. CODEN: JSACAT.

GI For diagram(s), see printed CA Issue.

AB 4-(N3-Adenyl)butyric acid (I) and 4-(N7-guanyl)butyric acid (II) are prepd. by the reaction of purines with .gamma.-butyrolactone (III). Thus, a mixt. of adenine and III is refluxed to give 4-(N9-adenyl)butyric acid (IV) and I (major product). Guanine gives 4-(N9-guanyl)butyric acid (V) and II (major product). Adenosine is treated with III to gibe I and IV, and II and V are obtained from guanosine. A mixt. of adenylic acid, III, and water is kept at 40.degree. to give IV.

L26 ANSWER 23 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 25477-96-7 REGISTRY
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 9-(Carboxymethyl)adenine ethyl ester
CN Ethyl 9-adeninylacetate
FS 3D CONCORD
MF C9 H11 N5 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

42 REFERENCES IN FILE CA (1967 TO DATE)
42 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:70226 Recognition Directed Site-Selective Chemical Modification of Molecularly Imprinted Polymers. Umpleby, Robert J., II; Rushton, Gregory T.; Shah, Ripal N.; Rampey, Andrew M.; Bradshaw, Jessica C.; Berch, John K., Jr.; Shimizu, Ken D. (Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC, 29208, USA). Macromolecules, 34(24), 8446-8452 (English) 2001. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

Searched by: Mary Hale 308-4258 CM-1 12D16

AB Demonstrated is the site-selective chem. modification (SSCM) of molecularly imprinted polymers (MIPs). In this strategy, MIPs are selectively chem. modified to improve the ratio of high-affinity to low-affinity binding sites and therefore the overall binding characteristics of the material. This was accomplished by preferentially eliminating the low-affinity binding sites by esterification with diazomethane or phenyldiazomethane. Selectivity in the esterification reaction was achieved using a guest mol. as an in situ protecting group that preferentially shields the high-affinity sites and leaves the low-affinity sites exposed toward reaction. The corresponding shifts in the populations of high- and low-affinity sites were quantified using affinity distribution anal., which quant. measures the heterogeneous distribution of binding sites in MIPs as no. of binding sites (N) with respect to binding affinity (K). Using affinity distribution anal., the SSCM strategy was shown to improve the percentage of high-affinity sites in a methacrylic acid (MAA)/ethylene glycol dimethacrylate (EGDMA) matrix, imprinted with Et adenine-9-acetate (EA9A) in acetonitrile. The effects of different solvents and concns. of guest mol. on the SSCM also were examd. The greatest improvements due to SSCM were obsd. when carried out in the imprinting solvent (acetonitrile). The demonstrated SSCM methodol. is complementary to existing strategies for improving MIPs and thus can be utilized in tandem to improve the binding characteristics of MIPs.

REFERENCE 2: 136:54011 PNA synthesis using a novel Boc/acyl protecting group strategy. Kofoed, Thomas; Hansen, Henrik F.; Orum, Henrik; Koch, Troels (PNA Diagnostics A/S, Copenhagen, Den.). Journal of Peptide Science, 7(8), 402-412 (English) 2001. CODEN: JPSIEI. ISSN: 1075-2617. Publisher: John Wiley & Sons Ltd..

AB The synthesis of novel Boc/acyl protected (Boc = tert-butoxycarbonyl) monomers for the synthesis of peptide nucleic acid (PNA) is described. The oligomerization protocol using these new monomers has been optimized with regard to coupling reagents. The use of base-labile acyl protecting groups at the exocyclic amines of the heterocyclic bases (isobutyryl for guanine and benzoyl for adenine and cytosine) and a PAM-linked solid support offers an attractive alternative to the present procedures used in PNA synthesis. This strategy has been applied for the synthesis of a test 17mer PNA on both control pore glass (CPG) and a polystyrene MBHA support and was used in the prepn. of PNA-DNA chimeras.

REFERENCE 3: 135:153391 Application of the Freundlich adsorption isotherm in the characterization of molecularly imprinted polymers. Umpleby, R. J.; Baxter, S. C.; Bode, M.; Berch, J. K.; Shah, R. N.; Shimizu, K. D. (Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC, 29208, USA). Analytica Chimica Acta, 435(1), 35-42 (English) 2001. CODEN: ACACAM. ISSN: 0003-2670. Publisher: Elsevier Science B.V..

AB The binding isotherm for a polymer molecularly imprinted with Et adenine-9-acetate was obsd. to obey the common Freundlich isotherm. To test the generality of the Freundlich isotherm with respect to molecularly imprinted polymers (MIPs), a survey of systems from the literature was conducted, revealing that the Freundlich isotherm gives a good math. approxn. of the binding characteristics for noncovalently imprinted polymers. The utility of the Freundlich isotherm in the calcn. of binding parameters, as well as its limitations and implication of an exponential distribution of binding sites in imprinted polymers were discussed.

REFERENCE 4: 134:353553 Preparation of double-stranded peptide nucleic acids. Norden, Benget; Wittung, Pernilla; Buchardt, Ole; Egholm, Michael; Nielsen, Peter E.; Berg, Rolf (Swed.). U.S. US 6228982 B1 20010508, 62 pp., Cont.-in-part of U.S. 5,539,082. (English). CODEN: USXXAM. APPLICATION: US 1993-88661 19930702. PRIORITY: WO 1992-EP1219 19920522; US 1993-54363 19930426.

Searched by: Mary Hale 308-4258 CM-1 12D16

AB A novel class of compds., known as peptide nucleic acids, form double-stranded structures with one another and with ssDNA. The peptide nucleic acids generally comprise ligands such as naturally occurring DNA bases attached to a peptide backbone through a suitable linker. Claimed is a compn. comprising two polymeric strands which are hydrogen bonded to each other. Each strand has the formula Q-C1-B1(A1-L1)-D1-G1-C2-B2(A2-L2)-D2-G2-Cn-Bn(An-Ln)-Dn-I [n is at least 2; each L1-Ln is independently selected from H, OH, (C1-C4)alkanoyl, (non)naturally occurring nucleobases, arom. moieties, DNA intercalators, nucleobase-binding groups, heterocyclic moieties, and reporter ligands; each C1-Cn and each D1-Dn is identical and has the formula (CR6R7)y and (CR6R7)z, resp., where each y and z is 0-10, the sum y + z being greater than 2 but not more than 10 and R6 is H and R7 is the side chain of a naturally occurring .alpha.-amino acid or R6 and R7 are H, alkyl, aryl, aralkyl, hydroxy, etc.; each G1-Gn-1 is identical and has the formula NR3CO, NR3CS, NR3SO or NR3SO2; each A1-An and each B1-Bn is identical, where A is (CR1R2)p-Y-(CR1R2)q (Z), Z-C(X) or Z-NR3CO (p, q = 0-5; Y is a single bond, O, S or NR4; X = O, S, Se, NR3, CH2, CMe2; R1-R4 = H, alkyl, alkoxy, hydroxy, amino, etc.) and B is N or R3N+ or A is Z-C(:X)NR3 and B is CH; Q is CO2H, CONR'R'', SO3H, SONR'R'' or an activated deriv. of CO2H or SO3H; I is NHR'''R'''' or NR'''C(O)R'''' (R', R'', R''' and R'''' are selected from H, alkyl, an amino protecting groups, reporter ligands, intercalators, chelators, peptides, proteins, carbohydrates, lipids, steroids, nucleosides, nucleotides, nucleotide diphosphates, nucleotide triphosphates, oligonucleotides, oligonucleosides and sol. and non-sol. polymers)]. Thus, prepn., binding and helix formation of complementary antiparallel PNA strands H-GTAGATCACT-LysNH2 and H-AGTGATCTAC-LysNH2 was studied. The CD spectra of the PNA 10-mers are almost vanishingly small, indicating that there is no preferred helical stacking of bases. However, a strong CD spectrum arises upon titrn. of one 10-mer with the complementary 10-mer, a satn. obtained at about 1:1 stoichiometry. The CD spectrum resembles that of .beta.-DNA, indicating a right-handed helix. It is believed that a PNA-PNA complex having no preferred helicity initially is formed. The kinetics by which this double-stranded structure reorganizes into a uniform, right-handed double helix has been monitored and the activation parameters for the process detd.

REFERENCE 5: 134:237838 Improved preparation of peptide nucleic acid (PNA) combinatorial libraries. Cook, Phillip Dan; Kiely, John; Sprankle, Kelly (Isis Pharmaceuticals, Inc., USA). U.S. US 6204326 B1 20010320, 32 pp., Cont.-in-part of U.S. 5,539,083. (English). CODEN: USXXAM. APPLICATION: US 1998-131270 19980807. PRIORITY: US 1994-200742 19940223.

AB New sub-monomer synthetic methods for the prepn. of peptide nucleic acid oligomeric structures are disclosed that provide for the synthesis of both predefined sequence peptide nucleic acid oligomers as well as random sequence peptide nucleic acid oligomers. Further these methods also provide for the incorporation of peptide nucleic acid units or strings of such units with amino acids or strings of amino acids in chimeric peptide nucleic acid-amino acid compds. Further disclosed are methods of making random libraries of peptide nucleic acids using the fully preformed monomers. Thus, a combinatorial library of chimeric peptide nucleic acid oligomers was prepd. using 1-[(N2-benzyloxycarbonyl-N6-benzyloxy-2-aminopurin-9-yl)acetyl]-3-oxomorpholine (I), 1-[(N6-benzyloxycarbonyladenin-9-yl)acetyl]-3-oxomorpholine (II), 1-[(N4-benzyloxycarbonylcytosin-1-yl)acetyl]-3-oxomorpholine (III), and 1-(thymin-1-ylacetyl)-2-oxomorpholine (IV), which involved coupling of IV to a MBHA resin, Mitsunobu reaction of the resulting resin-bound hydroxy adduct with (Boc)2NH using Ph3P and di-Et azodicarboxylate, random coupling of the resulting resin-bound peptide nucleic acid monomer with a mixt. of I, II, III, and IV followed by Mitsunobu reaction for converting the terminal hydroxy group to the terminal amine moieties, repeating the latter procedure for extension of backbone and addn. of further nucleoside

bases to complete the oligomer of the desired length, addn. of a peptide to the peptide nucleic acid unit using std. solid phase Merrifield peptide synthesis, and cleavage of peptide nucleic acid oligomers from the resin.

REFERENCE 6: 134:147169 Combinatorial libraries having aminodiol monomer subunits. Hebert, Normand (Isis Pharmaceuticals, Inc., USA). U.S. US 6184389 B1 20010206, 41 pp., Cont.-in-part of U.S. Ser. No. 179,970. (English). CODEN: USXXAM. APPLICATION: US 1995-483311 19950607. PRIORITY: US 1994-179970 19940111.

AB Combinatorial libraries are constructed to include aminodiol monomer subunits connected by phosphodiester, phosphorothioate, or phosphoramidate linking moieties. Combinatorial libraries of the invention feature a plurality of functional groups attached to backbone and phosphoramidate combinatorial sites.

REFERENCE 7: 133:296662 Synthons for synthesis and deprotection of peptide nucleic acids under mild conditions. Coull, James M.; Egholm, Michael; Hodge, Richard P.; Ismail, Mohamed; Rajur, Sharanappa B. (Perseptive Biosystems, Inc., USA). U.S. US 6133444 A 20001017, 50 pp., Cont.-in-part of Appl. No. PCT/US94/14742. (English). CODEN: USXXAM. APPLICATION: US 1995-487666 19950607. PRIORITY: US 1993-172695 19931222; WO 1994-US14742 19941222.

AB Novel purine PNA synthons having protecting groups which may be removed under mild conditions are disclosed. The PNA synthons are prepd. by coupling novel N-substituted nucleobase intermediates having a carbamate protection of the exocyclic amino group of the heterocycle to an amino-protected backbone or an amino protected backbone ester of the amino acid N-(2-aminoethyl)glycine. The resultant PNA synthons have orthogonal protection of the carbamate protected nucleobase and the amino protected backbone. The purine PNA synthons are useful in the synthesis of peptide nucleic acids (PNAs) and other oligomers such as PNA-DNA chimeras, and may be used in automated synthesizers. Thus, a soln. of N6-(benzhydryloxycarbonyl)-9-adenylacetic acid (QOH) in MeCN contg. N-methylmorpholine and pivaloyl chloride was combined with a suspension of FmocNHCH2CH2NRCH2CO2H (I; Fmoc = fluorenylmethoxycarbonyl, R = H) in MeCN-H2O contg. Et3N to afford 87.5% I (R = Q).

REFERENCE 8: 133:208845 Measurement of the continuous distribution of binding sites in molecularly imprinted polymers. Umpleby, Robert J., II; Bode, Miguel; Shimizu, Ken D. (Dep. Chem. Biochem., University of South Carolina, Columbia, SC, 29208, USA). Analyst (Cambridge, United Kingdom), 125(7), 1261-1265 (English) 2000. CODEN: ANALAO. ISSN: 0003-2654. Publisher: Royal Society of Chemistry.

AB Reported is the first affinity spectrum (AS) [no. of binding sites (N) vs. assocn. const. (K)] for a non-covalently imprinted polymer. The AS method yields the distribution of sites over a continuous range of binding consts. and characterizes the heterogeneity present in imprinted polymers better than current methodologies. To demonstrate the generality of the AS method, the distributions for three different imprinted polymers (two of which were taken from the literature) were calcd. from their resp. binding isotherms. The shapes of the distribution curves were different yet consistent with the resp. covalent or non-covalent imprinting mechanisms. Finally, the binding parameters derived from the AS method were compared with those detd. by the more common Scatchard anal. and were in general agreement.

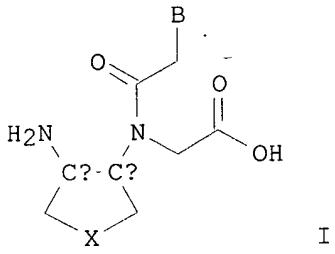
REFERENCE 9: 132:265495 Fmoc/Acyl protecting groups in the synthesis of polyamide (peptide) nucleic acid monomers. Timar, Zoltan; Kovacs, Lajos; Kovacs, Gyorgyi; Schmel, Zoltan (Department of Medicinal Chemistry, Albert Szent-Gyorgyi Medical University, Szeged, H-6720, Hung.). Perkin 1 (1), 19-26 (English) 2000. CODEN: PERKF9. Publisher: Royal Society of Chemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16

AB The chem. synthesis of polyamide (peptide) nucleic acid (PNA) monomers has been accomplished using Fmoc [N-(2-aminoethyl)glycine backbone], anisoyl (adenine), 4-tert-butylbenzoyl (cytosine) and isobutyryl/diphenylcarbamoyl (guanine) protecting-group combinations, thus allowing oligomer synthesis on both peptide and oligonucleotide synthesizers. An alternative method for the prepn. of (N6-anisoyladenin-9-yl)acetic acid is described using partial hydrolysis of a dianisoylated deriv. Different methods were studied for guanine alkylation including (a) Mitsunobu reaction; (b) low-temp., sodium hydride- and (c) N,N-diisopropylethylamine-mediated alkylation reactions to give preferentially N9-substituted derivs. Empirical rules are proposed for differentiating N9/N7-substituted guanines based on their 13C NMR chem.-shift differences.

REFERENCE 10: 131:351677 Preparation of chiral peptide nucleic acid monomers and oligomers. Nielsen, Peter; Buchardt, Ole; Lagriffoul, Pierre (Den.). U.S. US 5977296 A 19991102, 33 pp., Cont.-in-part of U.S. Ser. No. 108,591, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1994-366231 19941228. PRIORITY: DK 1991-986 19910524; DK 1991-987 19910524; DK 1992-510 19920415; WO 1992-EP1219 19920522; US 1992-108591 19920522.

GI



I

AB Peptide nucleic acid (PNA) monomers I [X = (CH2)n (n = 0, 1, 2, 3), B is a naturally or non-naturally occurring nucleobase, at least one of C.alpha. or C.beta. is in the S-configuration] were synthesized and applied to the synthesis of oligomers. Thus, N-2-(2S-Boc-aminocyclohex-1S-yl)-N-(thymin-1-ylacetyl)glycine (Boc-T**; Boc = tert-butoxy-carbonyl) was prepd. and incorporated into PNA oligomer H-TTTTT**TTTTT-Lys-NH2. Hybrids of H-TTTTT**TTTTT-Lys-NH2 (and the corresponding RR isomer) and AAAAAAAAAA or AAAACAAAAA were prepd. and their melting temps. compared with those of H-TTTTTTTTTT-Lys-NH2.

L26 ANSWER 24 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 23124-18-7 REGISTRY
CN 9H-Purine-9-butanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 9H-Purine-9-butyric acid, 6-amino-, methyl ester (8CI)
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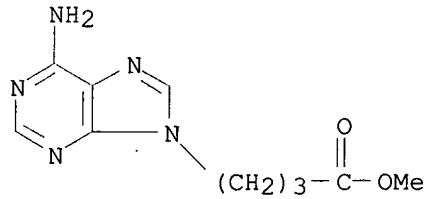
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16

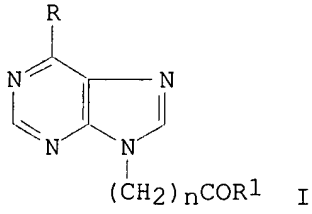


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 102:149749 Synthesis of modified amino acids containing purine bases of nucleic acids. Poritere, S.; Paegle, R.; Lidaks, M. (Inst. Org. Sint., Riga, 226006, USSR). Khim. Geterotsikl. Soedin. (1), 126-30 (Russian) 1985. CODEN: KGSSAQ. ISSN: 0453-8234.

GI



AB Adenylalkanoyl amino acids I [R = NH2, n = 1, 2, 3; R1 = NH(CH2)mCH(NH2)CO2H (m = 1-4), NH(CH2)mCO2H (m = 2, 3, 5), leucine, or phenylalanine residues] were prepd. from acids I (R1 = OH) via azides I (R1 = N3). Hypoxanthine analogs (I; R = OH, n = 1, 2; R1 = amino acid residue) were prepd. similarly.

REFERENCE 2: 71:49898 Syntheses of some 9-substituted adenines as inhibitors of adenosine deaminase. Chakraborti, S. K. (Chittaranjan Nat. Cancer Res. Centre, Calcutta, India). Indian J. Chem., 7(5), 426-9 (English) 1969. CODEN: IJOCAP.

GI For diagram(s), see printed CA Issue.

AB The syntheses of some adenines (I) (n = 1-3, R = CO2H, CO2Me, CN, NH2, CH2NH2, CO2C6H4NO2-p), as possible inhibitors of adenosine deaminase are described. Most of the compds. are either weakly inhibitory or non-inhibitory to adenosine deaminase.

L26 ANSWER 25 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 23124-10-9 REGISTRY
CN 9H-Purine-9-acetic acid, 6-amino-, methyl ester (8CI, 9CI) (CA INDEX NAME)
FS 3D CONCORD
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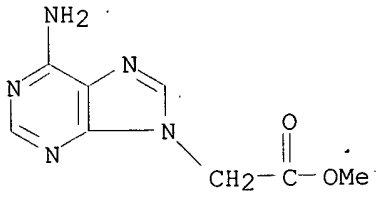
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1967 TO DATE)
9 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:371947 Design, Synthesis, and Biological Evaluation of Novel Nucleoside and Nucleotide Analogues as Agents against DNA Viruses and/or Retroviruses. Hakimelahi, Gholam Hossein; Ly, Tai Wei; Moosavi-Movahedi, Ali A.; Jain, Moti L.; Zakerinia, Maryam; Davari, Hady; Mei, Hui-Ching; Sambaiah, Thota; Moshfegh, Ali A.; Hakimelahi, Shahram (Institute of Chemistry, Academia Sinica, Taipei, 115, Taiwan). Journal of Medicinal Chemistry, 44(22), 3710-3720 (English) 2001. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A novel strategy was developed for the synthesis of N7-purine acyclic nucleosides. The key step involved the reaction between [2-(p-methoxyphenyloxy)ethoxy]methyl chloride and N9-tritylated nucleobases followed by concomitant self-detritylation. The N7-guanine acyclic nucleoside exhibited antiviral activity, but was phosphorylated by both HSV and Vero cell thymidine kinases; thus, it showed more potent cellular toxicity than acyclovir. The N7-adenine acyclic nucleoside was found to be an excellent antiviral agent as well as a good inhibitor of calf mucosal adenosine deaminase. This inhibitory property allows for a greater expression of antiviral activity of antiviral agents, such as N9-adenine acyclic nucleoside and ara-A. The N7-adenine acyclic nucleoside was phosphorylated neither by herpes simplex virus (HSV) thymidine kinase nor by Vero cell thymidine kinase, yet it enhanced the rate const. for the monophosphorylation of acyclovir by HSV thymidine kinase. Consequently, the combination of acyclovir and N7-adenine acyclic nucleoside exhibited greater antiviral activity than acyclovir alone. 7-[2-(Phosphonomethoxy)ethyl]adenine was also synthesized. The key step involved the reaction of 9-(2-cyanoethyl)adenine with Me iodoacetate in the presence of lithium 2,2,6,6-tetramethylpiperidine in THF. Unlike 9-[2-(phosphonomethoxy)ethyl]adenine (PMEA), the N7-isomer was not phosphorylated effectively by 5-phosphoribosyl 1-pyrophosphate synthetase (PRPP synthetase); thus, it did not exhibit pronounced antiviral activity. An adenine dinucleotide 5'-monophosphate I and its butenolide ester were also synthesized. Compd. I showed substrate activity toward PRPP synthetase and exhibited notable activity against DNA viruses. The antiviral activity of the butenolide ester deriv. was found to be higher than that of the parent mol. Compd. I is susceptible to degrdn. by snake venom and spleen phosphodiesterases. However, its resp. butenolide ester deriv. was completely resistant to snake venom and spleen enzymes. Guanine and adenine butenolide ester derivs. II (R1 = NH2, R2 = H; R1 = OH, R2 = NH2) were also synthesized and exhibited notable anti-DNA virus

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and anti-retrovirus activity in vitro. Final compds. were evaluated for their inhibitory effect on HSV-1-induced mortality in NMRI mice. The N7-adenine acyclic nucleoside [LD50 (i.p.) 950 mg/kg], the butenolide ester of I [LD50 (i.p.) 675 mg/kg], and II (R1 = NH2, R2 = H)[LD50 (i.p.) 710 mg/kg] were found to be potent anti-HSV-1 agents in vivo. In addn., II (R1 = NH2, R2 = H) efficiently decreased tumor formation induced by Moloney murine sarcoma virus (MSV) in NMRI mice while significantly increasing the survival time of MSV-infected mice.

REFERENCE 2: 129:216894 Solid-phase synthesis of peptide nucleic acid (PNA) monomers and their oligomerization using disulfide anchoring linkers. Aldrian-Herrada, Gudrun; Rabie, Alain; Wintersteiger, Reinhold; Brugidou, Jean (Karl-Franzens-Universitat, Graz, Austria). J. Pept. Sci., 4(4), 266-281 (English) 1998. CODEN: JPSIEI. ISSN: 1075-2617. Publisher: John Wiley & Sons Ltd..

AB A new simple solid-phase method has been developed for synthesizing Boc-protected peptide nucleic acid (PNA) monomers. An immobilized backbone was built on Expansin resin using an ester disulfide handle: 2-hydroxypropyl-dithio-2'-isobutyric acid (HPDI). The base acetic acids of thymine, Z-cytosine, Z-adenine, and 6-O-benzyl guanine were prepd. and coupled to the immobilized backbone. The HPDI handle was cleaved under mild conditions by cyanolysis or assisted hydrolysis with tris(2-carboxyethyl)phosphine (TCEP) to give undamaged PNA monomers. These monomers were coupled to form oligomers by the solid-phase method with another disulfide linkage: aminoethyldithio-2-isobutyric acid (AEDI) grafted on an amino-functionalized TentaGel resin, using in situ neutralization and TBTU as activating reagent. Final cleavage of the AEDI linker gave PNA bearing a cysteamide residue that could be useful for optimizing PNA properties. Oligomers of up to 16 residues long were assembled.

REFERENCE 3: 128:75666 Liquid phase synthesis of peptide nucleic acid (or polyamide nucleic acid) dimers. Farese, Audrey; Pairot, Sandrine; Patino, Nadia; Ravily, Veronique; Condom, Roger; Aumelas, Andre; Guedj, Roger (Laboratoire de Chimie Bio-Organique, CNRS ESA 6001, Universite de Nice Sophia-Antipolis, Nice, F-06108, Fr.). Nucleosides Nucleotides, 16(10 & 11), 1893-1906 (English) 1997. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Marcel Dekker, Inc..

AB The liq. phase synthesis of "polyamide nucleic acid" (PNA) dimers contg. the purine nucleic acid bases adenine and guanine has been achieved in good yields. This strategy was elaborated in order to circumvent difficult direct coupling of protected PNA monomers. This method can be applied to the liq. phase synthesis of short protected polyPNAs fragments, which can then selectively be deprotected.

REFERENCE 4: 126:118200 Improved synthons for the synthesis and deprotection of peptide nucleic acids under mild conditions. Coull, James M.; Egholm, Michael; Hodge, Richard P.; Ismail, Mohamed; Rajur, S. B. (Perseptive Biosystems, Inc., USA). PCT Int. Appl. WO 9640685 A1 19961219, 138 pp. DESIGNATED STATES: W: JP; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US9144 19960606. PRIORITY: US 1995-487666 19950607.

AB A method is disclosed for prepg. novel peptide nucleic acid (PNA) synthons having protecting groups capable of removal under mild conditions. The PNA synthons are prepd. by coupling novel N-substituted nucleobase intermediates having a carbamate protection of the exocyclic amino group of the heterocycle to an amino protected backbone or an amino protected backbone ester of the amino acid N-(2-aminoethyl)glycine. The resultant PNA synthons have orthogonal protection of the carbamate protected nucleobase and the amino protected backbone. Thus, a soln. of N6-(benzhydryloxycarbonyl)-9-adenylacetic acid (QOH) in MeCN contg. N-methylmorpholine and pivaloyl chloride was combined with a suspension of

FmocNHCH2CH2NRCH2CO2H (I; Fmoc = fluorenylmethoxycarbonyl, R = H) in MeCN-H2O contg. Et3N to afford 87.5% I (R = Q).

REFERENCE 5: 125:320771 Synthesis and properties of DNA-PNA chimeric oligomers. Finn, Patrick J.; Gibson, Neil J.; Fallon, Rachel; Hamilton, Alan; Brown, Tom (Dep. Chemistry, Univ. Southampton, Highfield, Southampton, SO17 1BJ, UK). Nucleic Acids Res., 24(17), 3357-3363 (English) 1996. CODEN: NARHAD. ISSN: 0305-1048.

AB Adenine, thymine and cytosine PNA (peptide nucleic acid) monomers have been prepd. using 3-amino-1,2-propanediol as a starting material. The benzoyl group was used to protect the exocyclic amines of the heterocyclic bases of A and C PNA monomers and the backbone primary amine was protected with the monomethoxytrityl group. The thymine and cytosine PNA monomers were used in conjunction with std. DNA synthesis monomers to produce chimeric PNA-DNA (PDC) oligomers. UV melting studies confirmed that these oligomers form stable hybrids with complementary DNA strands and that mismatches in the DNA but more so in the PNA sections lead to duplex destabilization.

REFERENCE 6: 124:290251 Liquid phase synthesis of a peptidic nucleic acid dimer. Farese, Audrey; Patino, Nadia; Condom, Roger; Dalleu, Sandrine; Guedj, Roger (Laboratoire Chimie Bioorganique, Univ. Nice Sophia-Antipolis, Nice, F-06108, Fr.). Tetrahedron Lett., 37(9), 1413-16 (English) 1996. CODEN: TELEAY. ISSN: 0040-4039.

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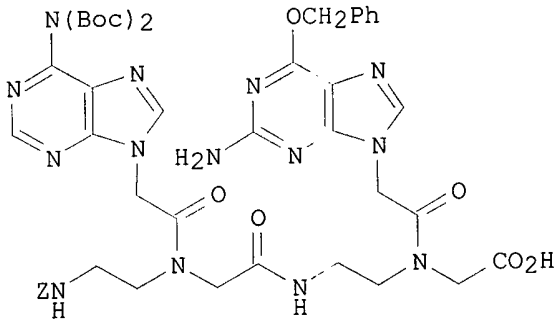

I

AB The first liq. phase synthesis of a peptide nucleic acid (PNA), dimer I (Boc = CO2CMe3, Z = PhCH2O2C) contg. guanine and adenine, has been achieved in good yields. A new strategy was elaborated in order to circumvent difficult coupling of the protected PNA.

REFERENCE 7: 102:160066 Studies on S-adenosyl-L-homocysteine hydrolase. XIV. Structure-activity studies on open-chain analogs of nucleosides: inhibition of S-adenosyl-L-homocysteine hydrolase and antiviral activity. 2. Acid open-chain analogs. Holy, Antonin; Votruba, Ivan; De Clercq, Erik (Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10/6, Czech.). Collect. Czech. Chem. Commun., 50(1), 262-79 (English) 1985. CODEN: CCCCAK. ISSN: 0366-547X.

AB Over 50 .omega.-carboxyalkyl derivs. of adenine and other purine bases were examd. for their inhibitory effects on rat liver S-adenosyl-L-homocysteine hydrolase (I) [9025-54-1] and their antiviral activity. To be a I inhibitor the analog must contain an adenine base substituted at position 9 by an .omega.-carboxyalkyl (C3-C5) chain bearing .gtoreq. 1 OH function. The abs. configuration at the side-chain is decisive for the dihydroxy and trihydroxy compds., but less important for the monohydroxyalkanoic acids. D-Eritadenine (II) [23918-98-1] and 3-(adenin-9-yl)-2-hydroxypropanoic acid (III) [94535-32-7] are the most

potent I inhibitors and the only compds. possessing antiviral activity (against vesicular stomatitis, parainfluenza type 3, reovirus type 1, and vaccinia virus). All these compds. effect a rapid irreversible inactivation of I. The esters of II and III exhibit little, if any inhibitory activity toward I; they are, however, much more potent antiviral agents than II and III, probably acting as prodrugs of the latter. 2-Amino-D-eritadenine [95973-21-0], (2R,3R)-5-(adenin-9-yl)-2,3-dihydroxypentanoic acid [95993-09-2], (9-(dicarboxymethyl)adenine [34573-03-0], 4-(adenin-9-yl)-2-hydroxybutanoic acid [53022-49-4], 3-(8-bromoadenin-9-yl)-2-hydroxypropanoic acid [95993-07-0], and O-carboxymethyl derivs. of 9-(2,3-dihydroxypropyl)- and 9-(2,3,4-trihydroxybutyl)adenine are described as novel compds.

REFERENCE 8: 97:163390 Studies on S-adenosyl-L-homocysteine hydrolase. Part V. Synthesis and antiviral activity of stereoisomeric eritadenines. Holy, Antonin; Votruba, Ivan; De Clercq, Erik (Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10/6, Czech.). Collect. Czech. Chem. Commun., 47(5), 1392-407 (English) 1982. CODEN: CCCCAK. ISSN: 0366-547X.

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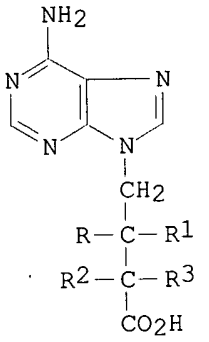
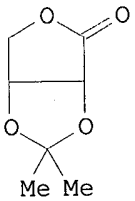


I, R=R2=OH, R1=R3=H
II, R=R2=H, R1=R3=OH
III, R=R3=H, R1=R2=OH
IV, R=R3=OH, R1=R2=H



V

AB Stereoisomeric eritadenines I-IV were prepd. by various methods, e.g., erythronolactone V was treated with adenine in Me2SO in the presence of K2CO3, the product was deprotected by acid hydrolysis and then chromatographed on Dowex 50 .times. 8 (H+ form) column to give 30% I. I and II were active against vaccinia, measles, and vesicular stomatitis virus; I was also effective against reo- and parainfluenza virus. In general the antiviral activity decreased in the order I > II .mchgt. III, IV.

REFERENCE 9: 71:49898 Syntheses of some 9-substituted adenines as inhibitors of adenosine deaminase. Chakraborti, S. K. (Chittaranjan Nat. Cancer Res. Centre, Calcutta, India). Indian J. Chem., 7(5), 426-9 (English) 1969. CODEN: IJOCAP.

GI For diagram(s), see printed CA Issue.

AB The syntheses of some adenines (I) (n = 1-3, R = CO2H, CO2Me, CN, NH2, CH2NH2, CO2C6H4NO2-p), as possible inhibitors of adenosine deaminase are described. Most of the compds. are either weakly inhibitory or non-inhibitory to adenosine deaminase.

L26 ANSWER 26 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 20128-29-4 REGISTRY
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 9-Carboxymethyladenine
CN Adenin-9-ylacetic acid

Searched by: Mary Hale 308-4258 CM-1 12D16

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CI COM
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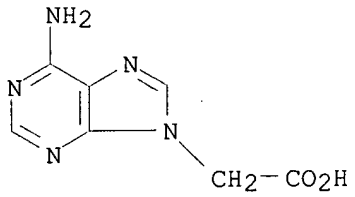
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1967 TO DATE)
14 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:5835 The self-assembly of calix[4]arene derivatives based on an A-T base pairing. Zeng, C.-C.; Tang, Y.-L.; Zheng, Q.-Y.; Huang, L.-J.; Xin, B.; Huang, Z.-T. (Institute of Chemistry, Center for Molecular Science, Chinese Academy of Sciences, Beijing, 100080, Peop. Rep. China). Tetrahedron Letters, 42(35), 6179-6181 (English) 2001. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB Calix[4]arene derivs. with one adenine or thymine sidearm have been synthesized and their self-assocn. characteristics which depend on solvent, temp. and concns. are described. Mainly Watson-Crick A-T base pairing in these systems was detected using 1H NMR and ESI-MS.

REFERENCE 2: 133:85826 Peptide nucleic acids rather than RNA may have been the first genetic molecule. Nelson, Kevin E.; Levy, Matthew; Miller, Stanley L. (Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0506, USA). Proceedings of the National Academy of Sciences of the United States of America, 97(8), 3868-3871 (English) 2000. CODEN: PNASA6. ISSN: 0027-8424. Publisher: National Academy of Sciences.

AB Numerous problems exist with the current thinking of RNA as the first genetic material. No plausible prebiotic processes have yet been demonstrated to produce the nucleosides or nucleotides or for efficient two-way nonenzymic replication. Peptide nucleic acid (PNA) is a promising precursor to RNA, consisting of N-(2-aminoethyl)glycine (AEG) and the adenine, uracil, guanine, and cytosine-N-acetic acids. However, PNA has not yet been demonstrated to be prebiotic. We show here that AEG is produced directly in elec. discharge reactions from CH4, N2, NH3, and H2O. Elec. discharges also produce ethylenediamine, as do NH4CN polymns. AEG is produced from the robust Strecker synthesis with ethylenediamine. The NH4CN polymn. in the presence of glycine leads to the adenine and guanine-N9-acetic acids, and the cytosine and uracil-N1-acetic acids are produced in high yield from the reaction of cyanoacetaldehyde with hydantoic acid, rather than urea. Preliminary expts. suggest that AEG may polymerize rapidly at 100.degree. to give the polypeptide backbone of PNA. The ease of synthesis of the components of PNA and possibility of polymn. of AEG reinforce the possibility that PNA may have been the first genetic material.

REFERENCE 3: 131:199968 Synthesis of two new chiral blocks for the construction of peptide nucleic acid (PNA). Zhang, Li Gang; Min, Ji Mei; Zhang, Li He (National Laboratory of Natural and Biomimetic Drugs, Beijing

Medical University, Beijing, 100083, Peop. Rep. China). Chinese Chemical Letters, 10(3), 195-198 (English) 1999. CODEN: CCLEE7. ISSN: 1001-8417. Publisher: Chinese Chemical Society.

AB Protected L- and D-lysine were used as starting materials to synthesize two new types of chiral blocks for the construction of PNA. Nucleobase was linked to the .alpha.-NH2 of lysine via -CH2C(O)- spacer in type I and -C(O)- in type II. The corresponding oligomers were constructed in soln.

REFERENCE 4: 128:23092 Oligonucleotides with 3-hydroxy-N-acetylprolinol as sugar substitute. Ceulemans, Griet; Van Aerschot, Arthur; Rozenski, Jef; Herdewijn, Piet (Laboratory of Medicinal Chemistry, Rega Institute for Medical Research, K.U. Leuven, Louvain, B-3000, Belg.). Tetrahedron, 53(44), 14957-14974 (English) 1997. CODEN: TETRAB. ISSN: 0040-4020. Publisher: Elsevier.

AB Fully modified oligonucleotides were synthesized from the 3-O-phosphoramidites of monomethoxytritylated trans-3-hydroxy-N-[(N6-benzoyladenin-9-yl)-acetyl]-prolinol [(2S,3R) and (2R,3S) series], trans-3-hydroxy-N-[(thymin-1-yl)-acetyl]-prolinol [(2S,3R) and (2R,3S) series], and cis-3-hydroxy-N-[(N6-benzoyl-adenin-9-yl)-acetyl]-L-prolinol (2R,3R). Remarkably, as well the L-trans (2R,3S) as the D-trans (2S,3R) all-adenine oligonucleotides are capable of hybridization with complementary DNA and RNA. With modified all-thymine trans-oligomers no complexation with natural nucleic acids was obsd. However, complex formation between two modified strands of the same sense of chirality does occur with formation of a triple stranded complex. The all-thymine oligonucleotides with trans-3-HO-N-acetylprolinol backbone are capable of hybridization with trans-4-HO-N-acetylprolinol oligoadenylates of the same enantiomeric form in both the D and the L series, and inversely, the all-adenine oligonucleotide with the trans-3-HO conformation hybridizes with the trans-4-HO oligothymidylates. While the former interactions have a triple stranded origin, the latter are 1:1 interactions. No interactions were noticed upon mixing oligonucleotide analogs of different sense of chirality. Modified mixed trans-3-HO A,T sequences display no hybridization with complementary nucleic acids, nor homocomplex formation. The L-cis all-adenine oligonucleotide hybridizes with its RNA complement. Several complexes were investigated by CD and microcalorimetry. In conclusion, the 3-hydroxy-N-acetylprolinol system represents an example of homochiral oligonucleotides built up from two enantiomeric forms and hybridizing both with natural nucleic acids.

REFERENCE 5: 127:346600 Photochemistry of 4-Thiothymine Derivatives in the Presence of N-9-Substituted-Adenine Derivatives: Formation of N-6-Formamidopyrimidines. Saintome, Carole; Clivio, Pascale; Favre, Alain; Fourrey, Jean-Louis (Institut de Chimie des Substances Naturelles, CNRS, Gif-sur-Yvette, 91198, Fr.). J. Org. Chem., 62(23), 8125-8130 (English) 1997. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

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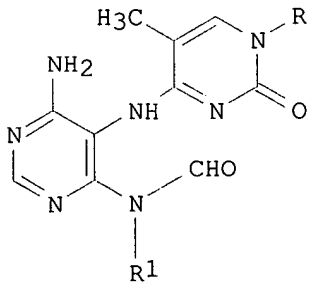


I

Searched by: Mary Hale 308-4258 CM-1 12D16

AB UV irradn. of aq. solns. contg. either 4-thiothymin-1-ylacetic acid (I) and adenosine (II), 4-thiothymidine (III) and adenin-9-ylacetic acid (IV), or I and IV led to 4,5-diamino-6-formamidopyrimidines, e.g. V (R = 2'-deoxyribofuranosyl, R1 = ribofuranosyl). These new observations demonstrate that the replacement of one or both nucleoside sugar residues by a carboxymethyl group does not affect the regioselective course of the photochem. reaction. The thermal decompn. of V that resulted from irradn. of III in the presence of II, was examd. along with its behavior under mild alk. conditions. This study is related to the mechanism of DNA damage caused by UV irradn. and formation of N-6-formamidopyrimidines.

REFERENCE 6: 126:271759 Pharmacokinetics and metabolism of selected prodrugs of PMEA in rats. Shaw, Jeng-Pyng; Louie, Michael S.; Krishnamurthy, V. V.; Arimilli, Murty N.; Jones, Robert J.; Bidgood, Alison M.; Lee, William A.; Cundy, Kenneth C. (Gilead Sciences, Inc., Foster City, CA, 94404, USA). Drug Metab. Dispos., 25(3), 362-366 (English) 1997. CODEN: DMDSAI. ISSN: 0090-9556. Publisher: Williams & Wilkins.

AB The oral bioavailability of PMEA (9-[2-(phosphonomethoxy)ethyl]adenine; adefovir) has been detd. in rats from three bis-ester prodrugs of PMEA: bis-(pivaloyloxymethyl) PMEA (bis-POM PMEA), bis-(phenyl) PMEA, and bis-(o-ethoxyphenyl) PMEA. The prodrugs were each administered to 9 male rats as solns. in PEG 400 at a dose of 10 mg-equiv. of PMEA per kg. Plasma samples were obtained over the course of 12 h and concns. of PMEA were detd. by fluorescence derivatization and anal. by HPLC. Concns. of PMEA obsd. in plasma following oral administration of PMEA prodrugs were compared with levels obsd. for i.v. PMEA. The obsd. oral bioavailabilities of PMEA from bis-POM PMEA, bis-(phenyl) PMEA, and bis-(o-ethoxyphenyl) PMEA were 38.2%, 2.46%, and 40.1%, resp. PMEA was the only metabolite formed after oral administration of bis-POM PMEA. Three metabolites were detected after oral administration of either bis-(phenyl) PMEA or bis-(o-ethoxyphenyl) PMEA to rats: PMEA, the corresponding monoester, and 2-adenylacetic acid. The major metabolite of bis-(phenyl) PMEA was 2-adenylacetic acid following oral administration. 2-Adenylacetic acid appears to have been formed from the intact prodrugs by a P 450 mediated oxidn. of the Et side chain.

REFERENCE 7: 102:160066 Studies on S-adenosyl-L-homocysteine hydrolase. XIV. Structure-activity studies on open-chain analogs of nucleosides: inhibition of S-adenosyl-L-homocysteine hydrolase and antiviral activity. 2. Acid open-chain analogs. Holy, Antonin; Votruba, Ivan; De Clercq, Erik (Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10/6, Czech.). Collect. Czech. Chem. Commun., 50(1), 262-79 (English) 1985. CODEN: CCCCAK. ISSN: 0366-547X.

AB Over 50 .omega.-carboxyalkyl derivs. of adenine and other purine bases were examd. for their inhibitory effects on rat liver S-adenosyl-L-homocysteine hydrolase (I) [9025-54-1] and their antiviral activity. To be a I inhibitor the analog must contain an adenine base substituted at position 9 by an .omega.-carboxyalkyl (C3-C5) chain bearing .gtoreq. 1 OH function. The abs. configuration at the side-chain is decisive for the dihydroxy and trihydroxy compds., but less important for the monohydroxyalkanoic acids. D-Eritadenine (II) [23918-98-1] and 3-(adenin-9-yl)-2-hydroxypropanoic acid (III) [94535-32-7] are the most potent I inhibitors and the only compds. possessing antiviral activity (against vesicular stomatitis, parainfluenza type 3, reovirus type 1, and vaccinia virus). All these compds. effect a rapid irreversible inactivation of I. The esters of II and III exhibit little, if any inhibitory activity toward I; they are, however, much more potent antiviral agents than II and III, probably acting as prodrugs of the latter. 2-Amino-D-eritadenine [95973-21-0], (2R,3R)-5-(adenin-9-yl)-2,3-dihydroxypentanoic acid [95993-09-2], (9-(dicarboxymethyl)adenine [34573-03-0], 4-(adenin-9-yl)-2-hydroxybutanoic acid [53022-49-4],

3-(8-bromoadenin-9-yl)-2-hydroxypropanoic acid [95993-07-0], and O-carboxymethyl derivs. of 9-(2,3-dihydroxypropyl)- and 9-(2,3,4-trihydroxybutyl)adenine are described as novel compds.

REFERENCE 8: 86:182968 Inhibitors of hypoxanthine metabolism in Ehrlich ascites tumor cells in vitro. Smith, Camilla M.; Zombor, George; Henderson, J. Frank (Cancer Res. Unit, Univ. Alberta, Edmonton, Alberta, Can.). Cancer Treat. Rep., 60(10), 1567-84 (English) 1976. CODEN: CTRRDO.

AB One hundred and sixty-one purine analogs and derivs. were tested for their ability to inhibit ten parameters of purine [120-73-0] metab. in Ehrlich ascites tumor cells incubated in vitro with radioactive hypoxanthine. Sixty-seven compds. were inhibitory against at least one parameter and 30 were inhibitory against two or more.

REFERENCE 9: 79:137090 Synthesis of carboxymethyl derivatives of purines and pyrimidines and their condensation with naturally occurring macromolecules. Jones, A. S.; Lewis, P.; Withers, S. F. (Chem. Dep., Univ. Birmingham, Birmingham, Engl.). Tetrahedron, 29(15), 2293-6 (English) 1973. CODEN: TETRAB.

AB 1-(Carboxymethyl)thymine (I), 1-(carboxymethyl)cytosine, and 9-(carboxymethyl)adenine (II) were prepd. from the appropriate bases and a Na haloacetate in alkali. Deamination of II with HNO2 gave 9-(carboxymethyl)hypoxanthine (III). 1-(Carboxymethyl)uracil, I, and III were condensed with protamine and dextran to give H2O-sol., base-substituted polymers. I-dextran showed a slow decrease in optical d. at 268 nm in 2 .times. SCC (SCC = 0.015M Na citrate, 0.015M NaCl) at 20.degree. of 30%. No decrease occurred in 7M urea. I-dextran gave an addnl. hypochromic effect with polyadenylic acid in 2 .times. SCC at 4.degree. and 14.degree. of 13 and 9% resp. The thymine-adenine residue ratio at max. hypochromicity was 3:1.

REFERENCE 10: 78:29824 9-Carboxymethyladenine. Takemoto, Kiichi; Kondo, Koichi (Chisso Co., Ltd.). Jpn. Kokai Tokkyo Koho JP 47030696 19721109 Showa, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1971-13923 19710313.

GI For diagram(s), see printed CA Issue.

AB The title compd. (I) was prepd. by hydrolysis and decarboxylation of dialkyl 9-adenylmalonate. E.g., 1.4 g di-Et 9-adenylmalonate in EtOH-H2O (1:3) was stirred 3 days with 0.3 g NaOH to give 0.15 g I.

L26 ANSWER 27 OF 29 REGISTRY COPYRIGHT 2002 ACS

RN 7083-40-1 REGISTRY

CN 9H-Purine-9-propanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)

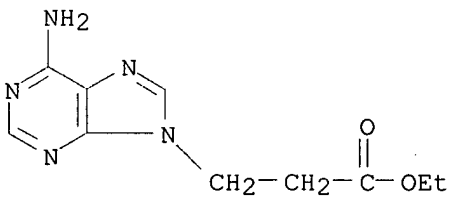
OTHER CA INDEX NAMES:

CN 9H-Purine-9-propionic acid, 6-amino-, ethyl ester (7CI, 8CI)

FS 3D CONCORD

MF C10 H13 N5 O2

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMINFORMRX
(*File contains numerically searchable property data)



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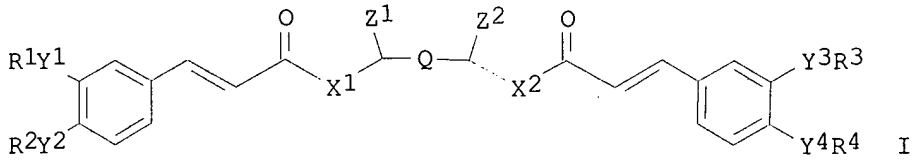
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1967 TO DATE)
8 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 133:296199 Preparation of acetylated and related analogs of chicoric acid as HIV integrase inhibitors. Burke, Terrence R.; Zhaiwei, Lin; Zhao, He; Neamati, Nouri; Pommier, Yves (Government of the United States of America as Represented by the Secretary, USA). PCT Int. Appl. WO 2000063152 A1 20001026, 76 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US4608 20000222. PRIORITY: US 1999-PV121127 19990222.

GI



I

AB Chicoric acid analogs I where: Q is a valence bond or CH2; X1 is O, NH, or CH2; X2 is O, NH, or CH2; Y1-Y4 are each a valence bond, O, or NH; where Y1-Y4 is a valence bond, the element R-R4 bonded to Y1-Y4 is a carboxy-contg. moiety selected from the group consisting of carboxymethyl, carboxyethyl, carboxypropyl, carboxy small alkyl and carboxy aryl; where Y1-Y4 is O, the element R-R4 bonded to Y-Y4 is each H, acetyl, propionyl, butyryl, or isobutyryl, or is a moiety forming a lower alkyl carbamate or an aryl carbamate; where Y-Y4 is NH, the element R1-R4 bonded to Y-Y4 is each acetyl, propionyl, butyryl, isobutyryl, small alkyl or aryl; Z1 and Z2 are each H, lower alkyl, CHO, CO2H, or CO2W, where W is lower alkyl or aryl, or, alternatively, where Q is a valence bond, Z1 and Z2, together with the adjacent carbon atoms and Q, form a ring structure, the carbon skeleton of the ring structure being selected from the group consisting of cyclohexane, cyclohexene, cyclopentane, cycloheptane, cycloheptene, and benzene; with the proviso that where each of Y-Y4 is O and all of R1-R4 are other than H, at least one of Z1 or Z2 is CO2H or CO2W; and with the proviso that where X1 and X2 are both O, Q is a valence bond, and Zi and Z2 are both CO2H, either at least one of R1-R4, is other than H or at least one of Y1-Y4 is other than O, were prepd. and have activity against HIV-1 integrase. The structural features that are required for this activity are elucidated by assaying these analogs and derivs. against HIV-1 integrase. Furthermore, methods of synthesis of the enantiomers of chicoric acid itself, as well as its analogs and derivs., are disclosed. Addnl., methods of use of chicoric acid analogs and derivs. to inhibit HIV-1 integrase are disclosed, as are compns. comprising chicoric acid analogs and derivs. Thus, N,O-bis-(3,4-dihydroxycinnamoyl)serine was prepd. and tested as HIV integrase inhibitor (IC50 = 3.3 .mu.M).

REFERENCE 2: 132:133869 Adenine-Uridine Base Pairing at the Water-Solid-Interface. Weisser, Michael; Kaeshammer, Josua; Menges,

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Bernhard; Matsumoto, Jin; Nakamura, Fumio; Ijiro, Kuniharu; Shimomura, Masatsugu; Mittler, Silvia (Max-Planck-Institut fuer Polymerforschung, Mainz, 55128, Germany). Journal of the American Chemical Society, 122(1), 87-95 (English) 2000. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB The formation of the base pair adenine-uracil at a water-solid interface, at an immobilized monolayer of adenine disulfide with adenine groups exposed to the very surface, resp., is shown here. To overcome the steric hindrance of tightly packed adenine groups in a pure adenine thiolate monolayer on gold, the formation of self-assembled monolayers out of a binary mixt. of the adenine disulfide and CH3- or OH-terminated thiols are investigated. Electro-chem. investigations, surface plasmon spectroscopy (PSP, plasmon surface polariton), multimode waveguide-PSP-coupling spectroscopy, contact angle measurements, and spontaneous desorption time-of-flight mass spectrometry were used to characterize the monolayers. The specific base pairing was investigated for a variety of monolayer compns. A specific base pairing was successful for an optimized mixed adenine/OH-terminated thiol monolayer. Nevertheless unspecific binding is a problem.

REFERENCE 3: 119:250359 Synthesis of adenine derivatives by solid-liquid phase-transfer catalysis. Wang, Zhicai; Lin, Dianwei; Zheng, Qihuang (Dep. Chem., Zhongshan Univ., Guangzhou, 510275, Peop. Rep. China). Yingyong Huaxue, 10(3), 42-6 (Chinese) 1993. CODEN: YIHUED.

AB Adenine derivs. eritadenine, Et 4-(6-amino-9H-purin-9-yl)-2(R),3(R)-dihydroxybutyrate, .beta.-adenylpropionic acid and Et .beta.-adenylpropionate have been synthesized from adenine by solid-liq. phase transfer catalysis. The effects of reaction conditions on the yields were studied. The results showed that PEG is a good phase transfer catalyst for the reaction.

REFERENCE 4: 119:226330 Preparation of PVA membrane containing nucleic acid analogs and studies on separation of nucleosides and dinucleotides using this membrane. Wada, Takehiko; Chirachianchai, Suwabun; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Mol. Cryst. Liq. Cryst. Sci. Technol., Sect. A, 219, 169-72 (English) 1992. CODEN: MCLCE9. ISSN: 1058-725X.

AB PVA membranes contg. nucleic acid analogs were prepd. Sepn. of nucleosides and dinucleotides were studied using these membranes. In the case of PVA membranes contg. thymine base, selective diffusion of adenosine, which is the complementary Watson-Crick base pair of thymine, was obsd. This may be caused by specific base-base interaction between thymine and adenine.

REFERENCE 5: 119:159963 Characterisation of adducts of nucleic bases and acrylic monomers. Crippa, Sergio; Di Gennaro, Patrizia; Lucini, Ruggero; Orlandi, Marco; Rindone, Bruno (Dip. Chim. Org. Ind., Univ. Milano, Milan, I-20133, Italy). Gazz. Chim. Ital., 123(4), 197-203 (English) 1993. CODEN: GCITA9. ISSN: 0016-5603.

AB Spectral data and thermodn. calcns. of adducts of guanine, adenine, thymine, and uracil with acrylonitrile, Et acrylate and Et crotonate are reported. Purine adducts derive from attack at N-7 and N-9, and pyrimidine adducts derive from attack at N-1. Acrylonitrile also forms N-1,N-3 bis adducts with pyrimidines. Structural assignment was by 1H and 13C NMR and using COSY-RELAY and NOE effects. Force-field calcns. indicated the most stable conformations of the reaction products.

REFERENCE 6: 114:207183 Synthesis and intramolecular cyclization of 5-aminoimidazolealkanoates and their conversion to purine derivatives. Birkett, Paul R.; Chapleo, Christopher B.; Mackenzie, Grahame (Humberside Coll. Higher Educ., Hull, HU6 7RT, UK). Synthesis (2), 157-9 (English) 1991. CODEN: SYNTBF. ISSN: 0039-7881.

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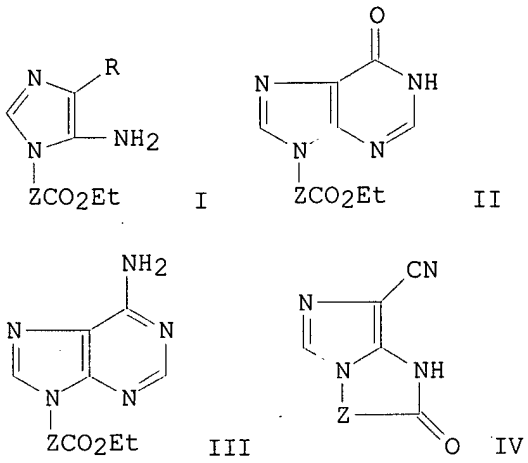

AB Reaction of EtOCH:NCHRCN (R = CONH2, cyano) with EtO2CZNH2.HCl [Z = CH2, CH2CH2, CHMe) in presence of Et3N gave 55-69% aminoimidazolylalkanoates I. Cyclization of I (R = CONH2) with HC(OEt)3 in DMF gave hypoxanthines II. Adenines III were obtained by the reaction of I (R = cyano) with HC(OEt)3 in EtOH, followed by 1 mol. equiv. NH3. Reaction of I (R = cyano) with ethanolic Et3N to give imidazoimidazoles or imidazopyrimidine IV (Z = CH2, CHMe, CH2CH2).

REFERENCE 7: 111:233438 Nucleic acid analogs for high-performance liquid chromatography. Inaki, Yoshiaki; Nagae, Suguru; Miyamoto, Takashi; Sugiura, Yoshihiko; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Polym. Sci. Technol. (Plenum), 38(Appl. Bioact. Polym. Mater.), 185-204 (English) 1988. CODEN: POSTB5. ISSN: 0093-6286.

AB Nucleic acid base and nucleoside derivs. were bonded to 3-aminopropyl-silanized silica (APS-silica) and silica gel. These resins were useful as the columns of high performance liq. chromatog. (HPLC) for the selective sepn. of oligoethylenimine derivs. having pendant thymine or adenine bases. These column systems were also applicable to the sepn. of nucleosides, nucleotides, and oligonucleotides.

REFERENCE 8: 102:149749 Synthesis of modified amino acids containing purine bases of nucleic acids. Poritere, S.; Paegle, R.; Lidaks, M. (Inst. Org. Sint., Riga, 226006, USSR). Khim. Geterotsikl. Soedin. (1), 126-30 (Russian) 1985. CODEN: KGSSAQ. ISSN: 0453-8234.

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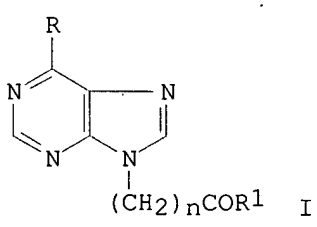

AB Adenylalkanoyl amino acids I [R = NH2, n = 1, 2, 3; R1 = NH(CH2)mCH(NH2)CO2H (m = 1-4), NH(CH2)mCO2H (m = 2, 3, 5), leucine, or

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phenylalanine residues] were prepd. from acids I (R1 = OH) via azides I (R1 = N3). Hypoxanthine analogs (I; R = OH, n = 1, 2; R1 = amino acid residue) were prepd. similarly.

L26 ANSWER 28 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 4323-13-1 REGISTRY
CN 9H-Purine-9-heptanoic acid, 6-amino- (7CI, 8CI, 9CI) (CA INDEX NAME)
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LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
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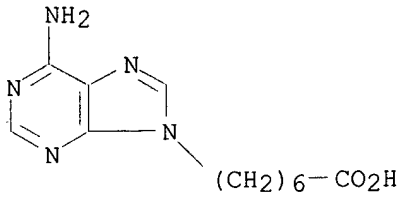

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 135:238179 Polymethylene derivatives of nucleic bases with .omega.-functional groups: II. Adenine and hypoxanthine derivatives. Makinsky, A. A.; Kritzyn, A. M.; Ul'yanova, E. A.; Zakharova, O. D.; Bugreev, D. V.; Nevinsky, G. A. (Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, 119991, Russia). Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya), 27(3), 167-172 (English) 2001. CODEN: RJBCET. ISSN: 1068-1620. Publisher: MAIK Nauka/Interperiodica.
AB N9-Polymethylene derivs. of adenine and hypoxanthine with various functional groups in the .omega.-position of the alkyl substituent were synthesized. Their physicochem. properties and effect on the HIV reverse transcriptase and DNA topoisomerase I were studied.

L26 ANSWER 29 OF 29 REGISTRY COPYRIGHT 2002 ACS
RN 4244-47-7 REGISTRY
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 9H-Purine-9-propionic acid, 6-amino- (7CI, 8CI)
OTHER NAMES:
CN 3-(6-Amino-9H-purin-9-yl)propionic acid
CN 3-(6-Aminopurin-9-yl)propionic acid
CN 9-(2-Carboxyethyl)adenine
FS 3D CONCORD
MF C8 H9 N5 O2
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER
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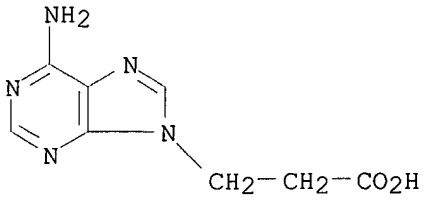
Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

31 REFERENCES IN FILE CA (1967 TO DATE)
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31 REFERENCES IN FILE CAPLUS (1967 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 135:180536 Internucleobase-Interaction-Directed Self-Assembly of Nanofibers from Homo- and Heteroditopic 1,.omega.-Nucleobase Bolaamphiphiles. Shimizu, Toshimi; Iwaura, Rika; Masuda, Mitsutoshi; Hanada, Takeshi; Yase, Kiyoshi (National Institute of Materials and Chemical Research, Tsukuba Ibaraki, 305-8565, Japan). Journal of the American Chemical Society, 123(25), 5947-5955 (English) 2001. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB The complementary 1,.omega.-thymine, 1,.omega.-adenine, and 1,.omega.-(thymine, adenine) bolaamphiphiles, [N,N'-bis[3-(2,4-dihydroxy-5-methylpyrimidine-1-yl)propionyl]1,n-diaminoalkane [T-n-T (n = 10, 11, 12)], N,N'-bis[3-(6-aminopurine-9-yl)propionyl]1,n-diaminoalkane [A-n-A (n = 10, 11, 12)], and N-[3-(2,4-dihydroxy-5-methylpyrimidine-1-yl)propionyl]-N'-[3-(6-aminopurine-9-yl)propionyl]1,n-diaminoalkane [T-n-A (n = 10, 11, 12)], resp.] have been synthesized. The spontaneous homo- and heteroassembly of these nucleobase-based bolaamphiphiles has been studied by light microscopy, energy-filtering transmission electron microscopy, FT-IR, and powder X-ray diffraction analyses. The achiral T-10-T bolaamphiphile produced in 10% ethanolic/aq. solns. unprecedented double-helical ropes of 1-2 .mu.m in widths and several hundred micrometers in length, whereas the complementary homolog A-10-A gave only microcryst. solids of 1-10 .mu.m in size. In contrast, an equimolar mixt. of T-10-T and A-10-A yielded supramol. fibers of 15-30 nm in width. 1H NMR, CD, and UV studies of soln. photoreactions of T-10-T suggested that under natural light the chiral rope formation is triggered by photodimerization of trace amts. of the thymine moieties in the T-10-T assemblies. Complementary hydrogen bond formation between the thymine-adenine heterobase pairs was found to prevent such a photoreaction and resulted in no chiral rope formation. The heteroditopic T-12-A bolaamphiphile self-assembled to form supramol. fibers. Multilamellar organization was proposed for the homo- and heteroassemblies made of T-n-T and A-n-A.

REFERENCE 2: 132:133869 Adenine-Uridine Base Pairing at the Water-Solid-Interface. Weisser, Michael; Kaeshammer, Josua; Menges, Bernhard; Matsumoto, Jin; Nakamura, Fumio; Ijiro, Kuniharu; Shimomura, Masatsugu; Mittler, Silvia (Max-Planck-Institut fuer Polymerforschung, Mainz, 55128, Germany). Journal of the American Chemical Society, 122(1), 87-95 (English) 2000. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB The formation of the base pair adenine-uracil at a water-solid interface, at an immobilized monolayer of adenine disulfide with adenine groups exposed to the very surface, resp., is shown here. To overcome the steric hindrance of tightly packed adenine groups in a pure adenine thiolate monolayer on gold, the formation of self-assembled monolayers out of a

binary mixt. of the adenine disulfide and CH3- or OH-terminated thiols are investigated. Electro-chem. investigations, surface plasmon spectroscopy (PSP, plasmon surface polariton), multimode waveguide-PSP-coupling spectroscopy, contact angle measurements, and spontaneous desorption time-of-flight mass spectrometry were used to characterize the monolayers. The specific base pairing was investigated for a variety of monolayer compns. A specific base pairing was successful for an optimized mixed adenine/OH-terminated thiol monolayer. Nevertheless unspecific binding is a problem.

REFERENCE 3: 130:38648 Preparation of double-headed nucleobase derivatives having higher alkylene bridging group. Shimizu, Toshimi; Iwaura, Ria; Masuda, Mitsutoshi (Agency of Industrial Sciences and Technology, Japan). Jpn. Kokai Tokkyo Koho JP 10298165 A2 19981110 Heisei, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1997-113711 19970501.

AB X(CH2)2CONH(CH2)nNHCO(CH2)2X (I; X = adenine residue, thymine residue; n = 10-12) are prepd. These compds. I have self-assembling property and Langmuir-Blodgett membranes or cryst. aggregates of which are useful for biosensors, electronic devices, etc. I (X = adenine residue) are prepd. by treatment of ACH2CH2CO2R2 (A = amino-protected adenine residue; R2 = CO2H-activating group) with H2N(CH2)nNH2 (II) and deprotection of amino-protecting group. I (X = thymine residue) are prepd. by treatment of TCH2CH2CO2R3 (T = thymine residue; R3 = CO2H-activating group) with II. A DMF soln. of p-nitrophenol 3-(6-trifluoroacetamidopurin-9-yl)propionate (prepn. given) was treated with imidazole and H2N(CH2)12NH2 at room temp. for 3 days to give 40% N,N'-bis[3-(6-trifluoroacetamidopurin-9-yl)propionyl]-1,12-diaminododecane, which was treated with H2O/MeOH soln. contg. K2CO3 under stirring overnight to give 93% N,N'-bis[3-(6-aminopurin-9-yl)propionyl]-1,12-diaminododecane.

REFERENCE 4: 129:189600 Base-specific interaction of polymers containing adenine: effect of chiral spacer on the interaction with polynucleotide. Inaki, Yoshiaki; Kamo, Shigeki; Miyata, Mikiji (Department of Materials and Life Science, Osaka University, Suita, 565, Japan). React. Funct. Polym., 37(1-3), 189-198 (English) 1998. CODEN: RFPOF6. ISSN: 1381-5148. Publisher: Elsevier Science B.V..

AB Polyethyleneimine derivs. of adenine with L- and D-serine as spacers were prepd. The polymer having D-serine spacer gave a stable polymer complex with poly(uridylic acid) (poly U), but the polymer having L-serine spacer gave an unstable polymer complex. The reason was concluded to be caused by the steric repulsion of L-serine units along the polymer chain when the polymer formed polymer complex with poly U.

REFERENCE 5: 126:60309 Thermodynamic effect of complementary hydrogen bond base pairing on aromatic stacking interaction in the guanine-X-Trp complex (X = adenine, guanine, cytosine, thymine). Tarui, Mariko; Nomoto, Noriko; Hasegawa, Yoko; Minoura, Katsuhiko; Doi, Mitsunobu; Ishida, Toshimasa (Dep. Physical Chem., Osaka Univ. Pharmaceutical Scis., Osaka, 569-11, Japan). Chem. Pharm. Bull., 44(11), 1998-2002 (English) 1996. CODEN: CPBTAL. ISSN: 0009-2363. Publisher: Pharmaceutical Society of Japan.

AB Four kinds of X-Trp-OH (X = adenine, guanine, cytosine, thymine) mols. were prepd. as model compds. to investigate the effect of complementary hydrogen bond base pairing on the stacking interaction of Trp with nucleic acid base. Assocn. consts. (Ka) of these compds. with two guanine derivs. (9-ethylguanine and 9-ethyl-7-methylguanine) were det. by Eadie-Hifstee plots of 1H-NMR titrn. expts., and the thermodn. parameters (.DELTA.H, .DELTA.S and .DELTA.G) for the resp. complexes were obtained by van't Hoff analyses based on the temp. dependence of the Ka values. The complexes were characterized by enthalpy/entropy compensations, where the interaction of cytosine-Trp with guanine derivs. was largely enthalpy-driven, accompanied by a small entropy component, whereas those of remaining complexes were all assocd. with a large increase in entropy,

accompanied by a small pos. enthalpy component. The present insight on the binding of increase in entropy, accompanied by a small pos. enthalpy component. The present insight on the binding of X-Trp with a guanine base provides a thermodn. basis for the importance of cooperative hydrogen bond pairing and arom. stacking interactions in the specific recognition of a nucleic acid base pair by protein.

REFERENCE 6: 119:250359 Synthesis of adenine derivatives by solid-liquid phase-transfer catalysis. Wang, Zhicai; Lin, Dianwei; Zheng, Qihuang (Dep. Chem., Zhongshan Univ., Guangzhou, 510275, Peop. Rep. China). Yingyong Huaxue, 10(3), 42-6 (Chinese) 1993. CODEN: YIHUED.

AB Adenine derivs. eritadenine, Et 4-(6-amino-9H-purin-9-yl)-2(R),3(R)-dihydroxybutyrate, .beta.-adenylpropionic acid and Et .beta.-adenylpropionate have been synthesized from adenine by solid-liq. phase transfer catalysis. The effects of reaction conditions on the yields were studied. The results showed that PEG is a good phase transfer catalyst for the reaction.

REFERENCE 7: 119:226330 Preparation of PVA membrane containing nucleic acid analogs and studies on separation of nucleosides and dinucleotides using this membrane. Wada, Takehiko; Chirachianchai, Suwabun; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Mol. Cryst. Liq. Cryst. Sci. Technol., Sect. A, 219, 169-72 (English) 1992. CODEN: MCLCE9. ISSN: 1058-725X.

AB PVA membranes contg. nucleic acid analogs were prepd. Sepn. of nucleosides and dinucleotides were studied using these membranes. In the case of PVA membranes contg. thymine base, selective diffusion of adenosine, which is the complementary Watson-Crick base pair of thymine, was obsd. This may be caused by specific base-base interaction between thymine and adenine.

REFERENCE 8: 114:43429 Synthesis and interaction of water-soluble nucleic acid analogs. Takemoto, Kiichi; Wada, Takehiko; Mochizuki, Eiko; Inaki, Yoshiaki (Fac. Eng., Osaka Univ., Osaka, Japan). Polym. Mater. Sci. Eng., 62, 558-62 (English) 1990. CODEN: PMSEDG. ISSN: 0743-0515.

AB Water sol. polyethyleneimine derivs. contg. both nucleic acid bases and homoserine were prepd. The polyethyleneimine derivs. formed 1:1 complex by complementary base pairing in aq. soln. These polymers also formed polymer complexes with polynucleotides by specific interaction between complementary nucleic acid bases.

REFERENCE 9: 113:59751 Orientation, recognition, and photoreaction of nucleolipids in model membranes. Ahlers, M.; Ringsdorf, H.; Rosemeyer, H.; Seela, F. (Inst. Org. Chem., Univ. Mainz, Mainz, 6500, Fed. Rep. Ger.). Colloid Polym. Sci., 268(2), 132-42 (English) 1990. CODEN: CPMSB6. ISSN: 0303-402X.

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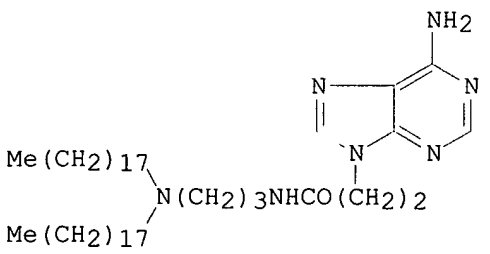

I

AB Amphiphiles with nucleobases and nucleosides as headgroups, e.g., I, have

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been synthesized. Their surface behavior was investigated in monolayers at the air/water interface. The double chain nucleolipids form stable monolayers with nearly identical surface pressure-area diagrams, whereas the spreading behavior of the mono chain amphiphiles is dominated by the various nucleobase-headgroups. When measuring the interactions between nucleolipid monolayers and nucleobases (monomeric and polymeric ones), specific base-base effects could be obsd.: the complementary nucleobases solubilized in the subphase expand the monolayer more than the non-complementary ones. Photodimerization reactions of thymine-amphiphiles were investigated in mono- and multilayers as well as in spin-coated films.

REFERENCE 10: 111:233438 Nucleic acid analogs for high-performance liquid chromatography. Inaki, Yoshiaki; Nagae, Suguru; Miyamoto, Takashi; Sugiura, Yoshihiko; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Polym. Sci. Technol. (Plenum), 38(Appl. Bioact. Polym. Mater.), 185-204 (English) 1988. CODEN: POSTB5. ISSN: 0093-6286.

AB Nucleic acid base and nucleoside derivs. were bonded to 3-aminopropyl-silanized silica (APS-silica) and silica gel. These resins were useful as the columns of high performance liq. chromatog. (HPLC) for the selective sepn. of oligoethylenimine derivs. having pendant thymine or adenine bases. These column systems were also applicable to the sepn. of nucleosides, nucleotides, and oligonucleotides.

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	989.67	989.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-16.52	-16.52

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FILE LAST UPDATED: 30 Apr 2002 (20020430/ED)

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Searched by: Mary Hale 308-4258 CM-1 12D16

L27 116 L26

=> d 11-116 cbib abs hitstr

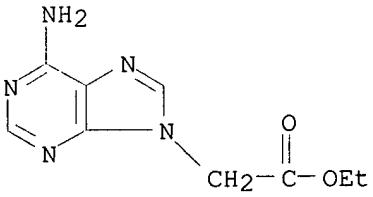
L27 ANSWER 11 OF 116 CAPLUS COPYRIGHT 2002 ACS
2001:195211 Document No. 134:237838 Improved preparation of peptide nucleic acid (PNA) combinatorial libraries. Cook, Phillip Dan; Kiely, John; Sprankle, Kelly (Isis Pharmaceuticals, Inc., USA). U.S. US 6204326 B1 20010320, 32 pp., Cont.-in-part of U.S. 5,539,083. (English). CODEN: USXXAM. APPLICATION: US 1998-131270 19980807. PRIORITY: US 1994-200742 19940223.

AB New sub-monomer synthetic methods for the prepn. of peptide nucleic acid oligomeric structures are disclosed that provide for the synthesis of both predefined sequence peptide nucleic acid oligomers as well as random sequence peptide nucleic acid oligomers. Further these methods also provide for the incorporation of peptide nucleic acid units or strings of such units with amino acids or strings of amino acids in chimeric peptide nucleic acid-amino acid compds. Further disclosed are methods of making random libraries of peptide nucleic acids using the fully preformed monomers. Thus, a combinatorial library of chimeric peptide nucleic acid oligomers was prepd. using 1-[(N2-benzyloxycarbonyl-N6-benzyloxy-2-aminopurin-9-yl)acetyl]-3-oxomorpholine (I), 1-[(N6-benzyloxycarbonyladenin-9-yl)acetyl]-3-oxomorpholine (II), 1-[(N4-benzyloxycarbonylcytosin-1-yl)acetyl]-3-oxomorpholine (III), and 1-(thymin-1-ylacetyl)-2-oxomorpholine (IV), which involved coupling of IV to a MBHA resin, Mitsunobu reaction of the resulting resin-bound hydroxy adduct with (Boc)2NH using Ph3P and di-Et azodicarboxylate, random coupling of the resulting resin-bound peptide nucleic acid monomer with a mixt. of I, II, III, and IV followed by Mitsunobu reaction for converting the terminal hydroxy group to the terminal amine moieties, repeating the latter procedure for extension of backbone and addn. of further nucleoside bases to complete the oligomer of the desired length, addn. of a peptide to the peptide nucleic acid unit using std. solid phase Merrifield peptide synthesis, and cleavage of peptide nucleic acid oligomers from the resin.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(improved prepn. of peptide nucleic acid (PNA) combinatorial libraries)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 12 OF 116 CAPLUS COPYRIGHT 2002 ACS
2001:91541 Document No. 134:147169 Combinatorial libraries having aminodiol monomer subunits. Hebert, Normand (Isis Pharmaceuticals, Inc., USA). U.S. US 6184389 B1 20010206, 41 pp., Cont.-in-part of U.S. Ser. No. 179,970. (English). CODEN: USXXAM. APPLICATION: US 1995-483311 19950607. PRIORITY: US 1994-179970 19940111.

AB Combinatorial libraries are constructed to include aminodiol monomer subunits connected by phosphodiester, phosphorothioate, or phosphoramidate linking moieties. Combinatorial libraries of the invention feature a plurality of functional groups attached to backbone and phosphoramidate

Searched by: Mary Hale 308-4258 CM-1 12D16

combinatorial sites.

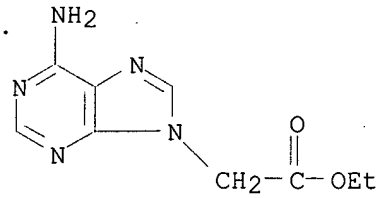
IT **25477-96-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(combinatorial libraries having aminodiol monomer subunits)

RN 25477-96-7 CAPLUS

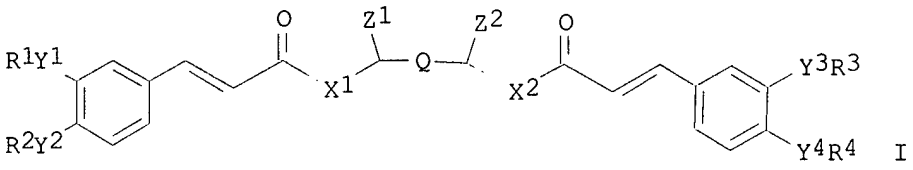
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 13 OF 116 CAPLUS COPYRIGHT 2002 ACS

2000:756659 Document No. 133:296199 Preparation of acetylated and related analogs of chicoric acid as HIV integrase inhibitors. Burke, Terrence R.; Zhaiwei, Lin; Zhao, He; Neamati, Nouri; Pommier, Yves (Government of the United States of America as Represented by the Secretary, USA). PCT Int. Appl. WO 2000063152 A1 20001026, 76 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US4608 20000222. PRIORITY: US 1999-PV121127 19990222.

GI



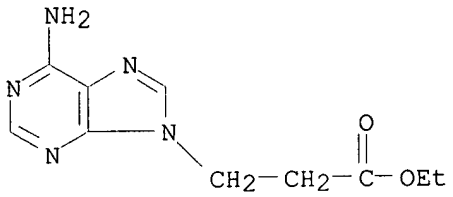
AB Chicoric acid analogs I where: Q is a valence bond or CH2; X1 is O, NH, or CH2; X2 is O, NH, or CH2; Y1-Y4 are each a valence bond, O, or NH; where Y1-Y4 is a valence bond, the element R-R4 bonded to Y1-Y4 is a carboxy-contg. moiety selected from the group consisting of carboxymethyl, carboxyethyl, carboxypropyl, carboxy small alkyl and carboxy aryl; where Y1-Y4 is O, the element R-R4 bonded to Y-Y4 is each H, acetyl, propionyl, butyryl, or isobutyryl, or is a moiety forming a lower alkyl carbamate or an aryl carbamate; where Y-Y4 is NH, the element R1-R4 bonded to Y-Y4 is each acetyl, propionyl, butyryl, isobutyryl, small alkyl or aryl; Z1 and Z2 are each H, lower alkyl, CHO, CO2H, or CO2W, where W is lower alkyl or aryl, or, alternatively, where Q is a valence bond, Z1 and Z2, together with the adjacent carbon atoms and Q, form a ring structure, the carbon skeleton of the ring structure being selected from the group consisting of cyclohexane, cyclohexene, cyclopentane, cycloheptane, cycloheptene, and

benzene; with the proviso that where each of Y-Y4 is O and all of R1-R4 are other than H, at least one of Z1 or Z2 is CO2H or CO2W; and with the proviso that where X1 and X2 are both O, Q is a valence bond, and Zi and Z2 are both CO2H, either at least one of R1-R4, is other than H or at least one of Y1-Y4 is other than O, were prepd. and have activity against HIV-1 integrase. The structural features that are required for this activity are elucidated by assaying these analogs and derivs. against HIV-1 integrase. Furthermore, methods of synthesis of the enantiomers of chicoric acid itself, as well as its analogs and derivs., are disclosed. Addnl., methods of use of chicoric acid analogs and derivs. to inhibit HIV-1 integrase are disclosed, as are compns. comprising chicoric acid analogs and derivs. Thus, N,O-bis-(3,4-dihydroxycinnamoyl)serine was prepd. and tested as HIV integrase inhibitor (IC50 = 3.3 .mu.M).

IT **7083-40-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of acetylated and related analogs of chicoric acid as hiv integrase inhibitors)

RN 7083-40-1 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 14 OF 116 CAPLUS COPYRIGHT 2002 ACS

2000:738892 Document No. 133:296662 Synthons for synthesis and deprotection of peptide nucleic acids under mild conditions. Coull, James M.; Egholm, Michael; Hodge, Richard P.; Ismail, Mohamed; Rajur, Sharanappa B. (Perseptive Biosystems, Inc., USA). U.S. US 6133444 A 20001017, 50 pp., Cont.-in-part of Appl. No. PCT/US94/14742. (English). CODEN: USXXAM. APPLICATION: US 1995-487666 19950607. PRIORITY: US 1993-172695 19931222; WO 1994-US14742 19941222.

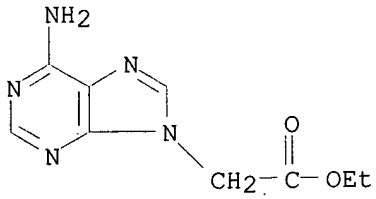
AB Novel purine PNA synthons having protecting groups which may be removed under mild conditions are disclosed. The PNA synthons are prepd. by coupling novel N-substituted nucleobase intermediates having a carbamate protection of the exocyclic amino group of the heterocycle to an amino-protected backbone or an amino protected backbone ester of the amino acid N-(2-aminoethyl)glycine. The resultant PNA synthons have orthogonal protection of the carbamate protected nucleobase and the amino protected backbone. The purine PNA synthons are useful in the synthesis of peptide nucleic acids (PNAs) and other oligomers such as PNA-DNA chimeras, and may be used in automated synthesizers. Thus, a soln. of N6-(benzhydryloxycarbonyl)-9-adenylacetic acid (QOH) in MeCN contg. N-methylmorpholine and pivaloyl chloride was combined with a suspension of FmocNHCH2CH2NRCH2CO2H (I; Fmoc = fluorenylmethoxycarbonyl, R = H) in MeCN-H2O contg. Et3N to afford 87.5% I (R = Q).

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthons for synthesis and deprotection of peptide nucleic acids under mild conditions)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

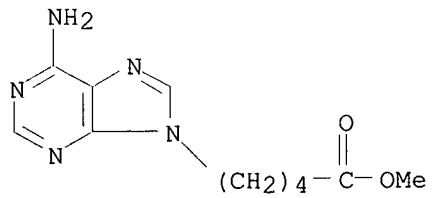


L27 ANSWER 15 OF 116 CAPLUS COPYRIGHT 2002 ACS
2000:671500 Document No. 134:178789 Synthesis of purine derivatives of potential immunomodulatory activity. Pini, E.; Rossi, E.; Ferraris, P. Cornaglia; Stradi, R. (Instituto di Chimica Organica-Facolta di Farmacia-Universita degli Studi di Milano, Milan, 20133, Italy). Bollettino Chimico Farmaceutico, 139(3), 107-113 (English) 2000. CODEN: BCFAAI. ISSN: 0006-6648. OTHER SOURCES: CASREACT 134:178789. Publisher: Societa Editoriale Farmaceutica.

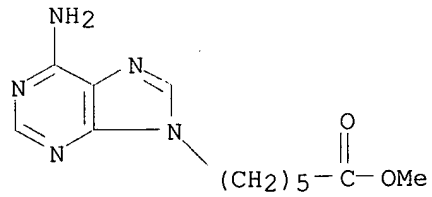
AB Moving from the interest as immunomodulatory agent of ST789 was studied the synthesis of series of N9-alkylated hypoxanthine and adenine. The synthesis and the chem. phys. properties of these derivs. are here described.

IT **326797-58-4P 326797-76-6P 326797-77-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of purine derivs. of potential immunomodulatory activity)

RN 326797-58-4 CAPLUS
CN 9H-Purine-9-pentanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)

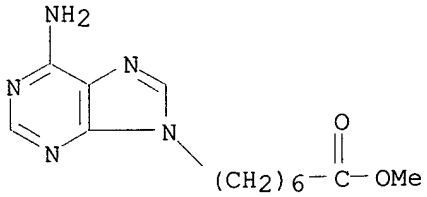


RN 326797-76-6 CAPLUS
CN 9H-Purine-9-hexanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)



RN 326797-77-7 CAPLUS
CN 9H-Purine-9-heptanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

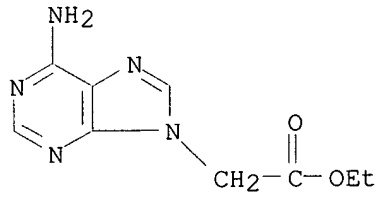


L27 ANSWER 16 OF 116 CAPLUS COPYRIGHT 2002 ACS
2000:440073 Document No. 133:208845 Measurement of the continuous distribution of binding sites in molecularly imprinted polymers. Umpleby, Robert J., II; Bode, Miguel; Shimizu, Ken D. (Dep. Chem. Biochem., University of South Carolina, Columbia, SC, 29208, USA). Analyst (Cambridge, United Kingdom), 125(7), 1261-1265 (English) 2000. CODEN: ANALAO. ISSN: 0003-2654. Publisher: Royal Society of Chemistry.

AB Reported is the first affinity spectrum (AS) [no. of binding sites (N) vs. assocn. const. (K)] for a non-covalently imprinted polymer. The AS method yields the distribution of sites over a continuous range of binding consts. and characterizes the heterogeneity present in imprinted polymers better than current methodologies. To demonstrate the generality of the AS method, the distributions for three different imprinted polymers (two of which were taken from the literature) were calcd. from their resp. binding isotherms. The shapes of the distribution curves were different yet consistent with the resp. covalent or non-covalent imprinting mechanisms. Finally, the binding parameters derived from the AS method were compared with those detd. by the more common Scatchard anal. and were in general agreement.

IT **25477-96-7**, Ethyl 9-adeninylacetate
RL: NUU (Other use, unclassified); USES (Uses)
(template; measurement of the continuous distribution of binding sites in molecularly imprinted polymers)

RN 25477-96-7 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 17 OF 116 CAPLUS COPYRIGHT 2002 ACS
2000:270332 Document No. 133:85826 Peptide nucleic acids rather than RNA may have been the first genetic molecule. Nelson, Kevin E.; Levy, Matthew; Miller, Stanley L. (Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0506, USA). Proceedings of the National Academy of Sciences of the United States of America, 97(8), 3868-3871 (English) 2000. CODEN: PNASA6. ISSN: 0027-8424. Publisher: National Academy of Sciences.

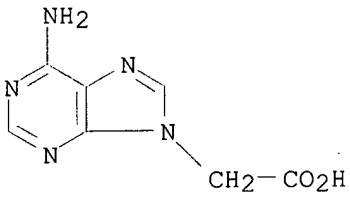
AB Numerous problems exist with the current thinking of RNA as the first genetic material. No plausible prebiotic processes have yet been demonstrated to produce the nucleosides or nucleotides or for efficient two-way nonenzymic replication. Peptide nucleic acid (PNA) is a promising precursor to RNA, consisting of N-(2-aminoethyl)glycine (AEG) and the adenine, uracil, guanine, and cytosine-N-acetic acids. However, PNA has

not yet been demonstrated to be prebiotic. We show here that AEG is produced directly in elec. discharge reactions from CH4, N2, NH3, and H2O. Elec. discharges also produce ethylenediamine, as do NH4CN polymns. AEG is produced from the robust Strecker synthesis with ethylenediamine. The NH4CN polymn. in the presence of glycine leads to the adenine and guanine-N9-acetic acids, and the cytosine and uracil-N1-acetic acids are produced in high yield from the reaction of cyanoacetaldehyde with hydantoic acid, rather than urea. Preliminary expts. suggest that AEG may polymerize rapidly at 100.degree. to give the polypeptide backbone of PNA. The ease of synthesis of the components of PNA and possibility of polymn. of AEG reinforce the possibility that PNA may have been the first genetic material.

IT **20128-29-4P**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(role of PNA in prebiotic mol. evolution)

RN 20128-29-4 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 18 OF 116 CAPLUS COPYRIGHT 2002 ACS

2000:161804 Document No. 133:2125 FT-SERS Studies on Molecular Recognition Capabilities of Monolayers of Novel Nucleolipid Amphiphiles. Huang, Jianguo; Li, Chun; Liang, Yingqiu (State Key Laboratory of Coordination Chemistry and Institute of Mesoscopic Solid State Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China). Langmuir, 16(8), 3937-3940 (English) 2000. CODEN: LANGD5. ISSN: 0743-7463. Publisher: American Chemical Society.

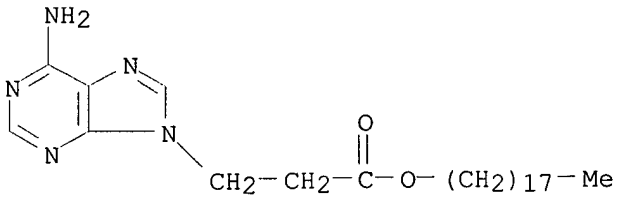
AB The mol. recognition effect in nucleic acids was simulated in the monolayers formed by six novel nucleolipid amphiphiles. Fourier transform surface-enhanced Raman scattering (FT-SERS) technique was introduced into the research area of mol. recognition occurring in an interface system. High-quality FT-SERS spectra of a single Langmuir-Blodgett (LB) monolayer of the nucleolipid amphiphiles were obtained. Characteristic vibrational modes of the corresponding complementary nucleic acid bases, which transferred along with the monolayers of nucleolipid amphiphiles into the LB films, were clearly seen. The mechanism of mol. recognition through multiple hydrogen bonds between complementary bases was described. It was proved that this technique can be used as a powerful tool for studying mol. recognition in interface systems because of its high sensitivity.

IT **188524-32-5**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(FT-SERS studies on mol. recognition capabilities of monolayers of novel nucleolipid amphiphiles)

RN 188524-32-5 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino-, octadecyl ester (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

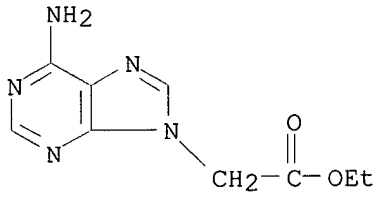


L27 ANSWER 19 OF 116 CAPLUS COPYRIGHT 2002 ACS
2000:119111 Document No. 132:265495 Fmoc/Acyl protecting groups in the synthesis of polyamide (peptide) nucleic acid monomers. Timar, Zoltan; Kovacs, Lajos; Kovacs, Gyorgyi; Schmel, Zoltan (Department of Medicinal Chemistry, Albert Szent-Gyorgyi Medical University, Szeged, H-6720, Hung.). Perkin 1 (1), 19-26 (English) 2000. CODEN: PERKF9. Publisher: Royal Society of Chemistry.

AB The chem. synthesis of polyamide (peptide) nucleic acid (PNA) monomers has been accomplished using Fmoc [N-(2-aminoethyl)glycine backbone], anisoyl (adenine), 4-tert-butylbenzoyl (cytosine) and isobutyryl/diphenylcarbamoyl (guanine) protecting-group combinations, thus allowing oligomer synthesis on both peptide and oligonucleotide synthesizers. An alternative method for the prepn. of (N6-anisoyladenin-9-yl)acetic acid is described using partial hydrolysis of a dianisoylated deriv. Different methods were studied for guanine alkylation including (a) Mitsunobu reaction; (b) low-temp., sodium hydride- and (c) N,N-diisopropylethylamine-mediated alkylation reactions to give preferentially N9-substituted derivs. Empirical rules are proposed for differentiating N9/N7-substituted guanines based on their 13C NMR chem.-shift differences.

IT **25477-96-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(protecting groups in the synthesis of polyamide peptide nucleic acid monomers)

RN 25477-96-7 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



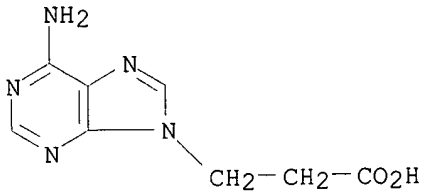
L27 ANSWER 20 OF 116 CAPLUS COPYRIGHT 2002 ACS
1999:799931 Document No. 132:133869 Adenine-Uridine Base Pairing at the Water-Solid-Interface. Weisser, Michael; Kaeshammer, Josua; Menges, Bernhard; Matsumoto, Jin; Nakamura, Fumio; Ijiro, Kuniharu; Shimomura, Masatsugu; Mittler, Silvia (Max-Planck-Institut fuer Polymerforschung, Mainz, 55128, Germany). Journal of the American Chemical Society, 122(1), 87-95 (English) 2000. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB The formation of the base pair adenine-uracil at a water-solid interface, at an immobilized monolayer of adenine disulfide with adenine groups exposed to the very surface, resp., is shown here. To overcome the steric hindrance of tightly packed adenine groups in a pure adenine thiolate monolayer on gold, the formation of self-assembled monolayers out of a binary mixt. of the adenine disulfide and CH3- or OH-terminated thiols are

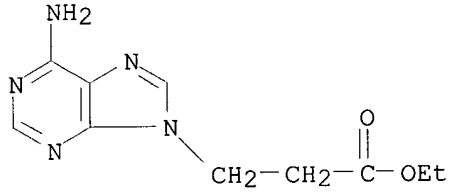
investigated. Electro-chem. investigations, surface plasmon spectroscopy (PSP, plasmon surface polariton), multimode waveguide-PSP-coupling spectroscopy, contact angle measurements, and spontaneous desorption time-of-flight mass spectrometry were used to characterize the monolayers. The specific base pairing was investigated for a variety of monolayer compns. A specific base pairing was successful for an optimized mixed adenine/OH-terminated thiol monolayer. Nevertheless unspecific binding is a problem.

IT **4244-47-7P 7083-40-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(adenine-uridine base pairing at the water-solid-interface)

RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)

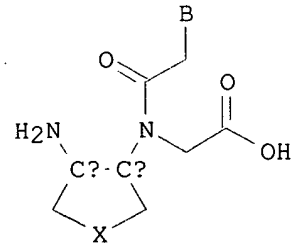


RN 7083-40-1 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 21 OF 116 CAPLUS COPYRIGHT 2002 ACS
1999:705034 Document No. 131:351677 Preparation of chiral peptide nucleic acid monomers and oligomers. Nielsen, Peter; Buchardt, Ole; Lagriffoul, Pierre (Den.). U.S. US 5977296 A 19991102, 33 pp., Cont.-in-part of U.S. Ser. No. 108,591, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1994-366231 19941228. PRIORITY: DK 1991-986 19910524; DK 1991-987 19910524; DK 1992-510 19920415; WO 1992-EP1219 19920522; US 1992-108591 19920522.

GI



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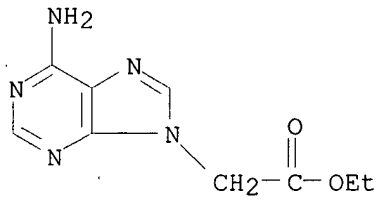
Searched by: Mary Hale 308-4258 CM-1 12D16

AB Peptide nucleic acid (PNA) monomers I [X = (CH2)n (n = 0, 1, 2, 3), B is a naturally or non-naturally occurring nucleobase, at least one of C.alpha. or C.beta. is in the S-configuration] were synthesized and applied to the synthesis of oligomers. Thus, N-2-(2S-Boc-aminocyclohex-1S-yl)-N-(thymin-1-ylacetyl)glycine (Boc-T**; Boc = tert-butoxy-carbonyl) was prepd. and incorporated into PNA oligomer H-TTTTT**TTTTT-Lys-NH2. Hybrids of H-TTTTT**TTTTT-Lys-NH2 (and the corresponding RR isomer) and AAAAAAAAAA or AAAACAAAAA were prepd. and their melting temps. compared with those of H-TTTTTTTTT-Lys-NH2.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of chiral peptide nucleic acid monomers and oligomers)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 22 OF 116 CAPLUS COPYRIGHT 2002 ACS

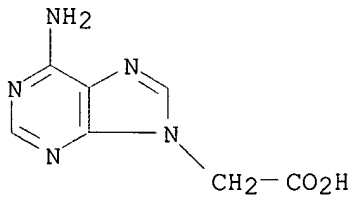
1999:446484 Document No. 131:199968 Synthesis of two new chiral blocks for the construction of peptide nucleic acid (PNA). Zhang, Li Gang; Min, Ji Mei; Zhang, Li He (National Laboratory of Natural and Biomimetic Drugs, Beijing Medical University, Beijing, 100083, Peop. Rep. China). Chinese Chemical Letters, 10(3), 195-198 (English) 1999. CODEN: CCLEE7. ISSN: 1001-8417. Publisher: Chinese Chemical Society.

AB Protected L- and D-lysine were used as starting materials to synthesize two new types of chiral blocks for the construction of PNA. Nucleobase was linked to the .alpha.-NH2 of lysine via -CH2C(O)- spacer in type I and -C(O)- in type II. The corresponding oligomers were constructed in soln.

IT **20128-29-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of two new chiral blocks for construction of peptide nucleic acid (PNA))

RN 20128-29-4 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 23 OF 116 CAPLUS COPYRIGHT 2002 ACS

1999:283238 Document No. 131:45036 Acyclic nucleotide analogs based on phosphonic acids. Efimtseva, E. V.; Mikhailov, S. N.; Fomicheva, M. V.; Meshkov, S. V.; Rodionov, M. S.; Khomutov, A. R.; De Clercq, E.

Searched by: Mary Hale 308-4258 CM-1 12D16

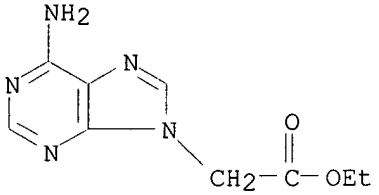
(Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, 117984, Russia). Bioorganicheskaya Khimiya, 24(1), 16-20 (Russian) 1998. CODEN: BIKHD7. ISSN: 0132-3423. Publisher: MAIK Nauka.

AB The synthesis of novel nucleotide analogs based on ethyl-phosphonic acids is described. A rigid structural element, an amide or a double bond, was characteristic of the compds. synthesized. The antiviral and cytotoxic activities of these compds. were studied in cell cultures.

IT **25477-96-7P**, 9-(Carboxymethyl)adenine ethyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(acyclic nucleotide analogs based on phosphonic acids)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 24 OF 116 CAPLUS COPYRIGHT 2002 ACS

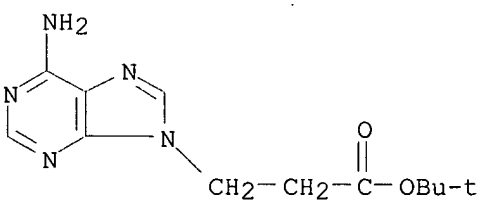
1999:217970 Document No. 130:296947 Synthesis of acyclic carba-nucleoside phosphonates, structural analogs to natural deoxyribonucleotides. Esposito, Annamaria; Perino, Maria Grazia; Taddei, Maurizio (Dipartimento Chimica, Universita Sassari, Sassari, I-07100, Italy). Eur. J. Org. Chem. (4), 931-936 (English) 1999. CODEN: EJOCFK. ISSN: 1434-193X. OTHER SOURCES: CASREACT 130:296947. Publisher: Wiley-VCH Verlag GmbH.

AB Acyclic carba-nucleoside phosphonates, modeled on natural deoxyribonucleotides were prepd. starting from DNA nucleobases and tert-Bu acrylate. The products obtained from a Michael-type reaction were elongated to .beta.-oxo esters that were first reduced to .beta.-hydroxy esters and then transformed into protected .beta.-hydroxy aldehydes. Wittig-Horner-Emmons reaction with the anion of CH2[PO(OCHMe2)2]2 gave, after deprotection, the desired 4-hydroxy-6-purinyl- or -6-pyrimidinyl-1-hexenylphosphonates. A dimer, potential precursor of acyclic polynucleotides (APN), homomorphous with DNA, was also prepd.

IT **223409-15-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of acyclic carba-nucleoside phosphonates as deoxyribonucleotide analogs)

RN 223409-15-2 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



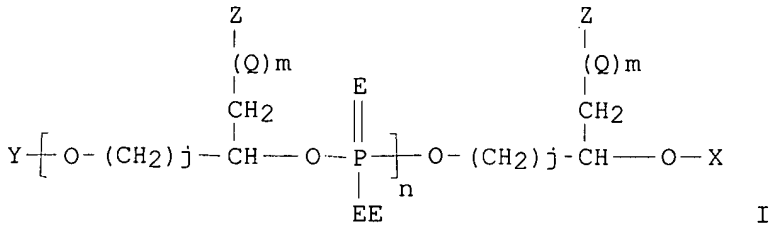
L27 ANSWER 25 OF 116 CAPLUS COPYRIGHT 2002 ACS

1999:205354 Document No. 130:237811 Preparation of ethylene glycol phosphate

Searched by: Mary Hale 308-4258 CM-1 12D16

linked oligodeoxyribonucleotides as phospholipase A2 inhibitors. Cook, Phillip Dan; Acevedo, Oscar L.; Davis, Peter W.; Ecker, David J.; Hebert, Normand (ISIS Pharmaceuticals, Inc., USA). U.S. US 5886177 A 19990323, 39 pp., Cont.-in-part of U.S. Ser. No. 179,970. (English). CODEN: USXXAM. APPLICATION: US 1996-669506 19960808. PRIORITY: US 1994-179970 19940111; WO 1995-US449 19950111.

GI



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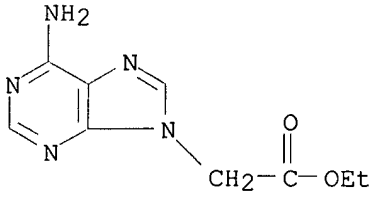
AB Novel ethylene glycol compds. I wherein; X is H, a phosphate group, phosphite group, a solid support, an oligodeoxyribonucleotide; Y is H, a hydroxyl protecting group, an oligodeoxyribonucleotide; E is O or S; EE is OH or amine; Q is alkyl, alkynyl, alkenyl, carbocycloalkyl, heterocycle; Z is alkyl, alkenyl, alkynyl, aminoalkyl,, aryl, aralkyl; m is 0, 1; n is 1-50; j is 1-6, are used to prep. oligodeoxyribonucleotides. The ethylene glycol monomers can be joined via std. phosphate linkages including phosphorothioate, phosphodiester, and phosphoramidate linkages. Useful functional groups include nucleobases as well as polar groups, hydrophobic groups, ionic groups, arom. groups and/or groups that participate in hydrogen-bonding. Thus, 1-[1-(N4-Benzoyl)cytosine]-3-O-dimethoxytrityl-2-O-[(N,N-diisopropylamino)-2-cyanoethoxyphosphite]propane was prepd. and used in synthesis of ethylene glycol phosphate linked oligodeoxyribonucleotides as phospholipase A2 inhibitors.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of ethylene glycol phosphate linked oligodeoxyribonucleotides as phospholipase A2 inhibitors)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 26 OF 116 CAPLUS COPYRIGHT 2002 ACS

1998:793060 Document No. 130:57170 Liposomal conjugated peptide nucleic acids having enhanced cellular uptake. Nielsen, Peter E.; Knudsen, Helle (Isis Pharmaceuticals,, Inc., USA). PCT Int. Appl. WO 9853801 A1 19981203, 60 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA,

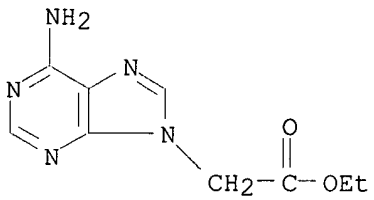
UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US10804 19980528. PRIORITY: US 1997-864765 19970528.

AB Peptide nucleic acids conjugated to lipophilic groups and incorporated into liposomes exhibit enhanced cellular uptake and distribution. Cellular uptake and distribution of peptide nucleic acids also increases with the introduction of an amino acid side chain into the backbone of peptide nucleic acids. Methods of modulating cellular uptake and methods for treating animals are provided. The peptide nucleic acids of the invention comprise naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(liposomal conjugated peptide nucleic acids having enhanced cellular uptake)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 27 OF 116 CAPLUS COPYRIGHT 2002 ACS

1998:724193 Document No. 130:38648 Preparation of double-headed nucleobase derivatives having higher alkylene bridging group. Shimizu, Toshimi; Iwaura, Ria; Masuda, Mitsutoshi (Agency of Industrial Sciences and Technology, Japan). Jpn. Kokai Tokkyo Koho JP 10298165 A2 19981110 Heisei, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1997-113711 19970501.

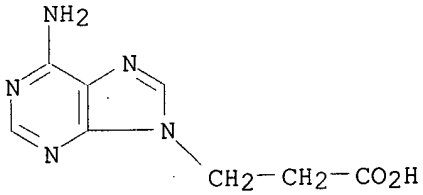
AB X(CH2)2CONH(CH2)nNHCO(CH2)2X (I; X = adenine residue, thymine residue; n = 10-12) are prepd. These compds. I have self-assembling property and Langmuir-Blodgett membranes or cryst. aggregates of which are useful for biosensors, electronic devices, etc. I (X = adenine residue) are prepd. by treatment of ACH2CH2CO2R2 (A = amino-protected adenine residue; R2 = CO2H-activating group) with H2N(CH2)nNH2 (II) and deprotection of amino-protecting group. I (X = thymine residue) are prepd. by treatment of TCH2CH2CO2R3 (T = thymine residue; R3 = CO2H-activating group) with II. A DMF soln. of p-nitrophenol 3-(6-trifluoroacetamidopurin-9-yl)propionate (prepn. given) was treated with imidazole and H2N(CH2)12NH2 at room temp. for 3 days to give 40% N,N'-bis[3-(6-trifluoroacetamidopurin-9-yl)propionyl]-1,12-diaminododecane, which was treated with H2O/MeOH soln. contg. K2CO3 under stirring overnight to give 93% N,N'-bis[3-(6-aminopurin-9-yl)propionyl]-1,12-diaminododecane.

IT **4244-47-7P**, 9-(2-Carboxyethyl)adenine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of self-assembling double-headed nucleobase derivs. having higher alkylene bridging group useful for biosensors and electronic materials)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16



L27 ANSWER 28 OF 116 CAPLUS COPYRIGHT 2002 ACS
1998:719165 Document No. 129:331055 Improved preparation of oligomeric peptide nucleic acid (PNA) combinatorial libraries. Cook, Phillip Dan; Kiely, John; Sprankle, Kelly (Isis Pharmaceuticals Inc, USA). U.S. US 5831014 A 19981103, 33 pp. Cont.-in-part of U.S. 5,539,083. (English). CODEN: USXXAM. APPLICATION: US 1996-693144 19960813. PRIORITY: US 1994-200742 19940223; WO 1995-US2182 19950222.

GI

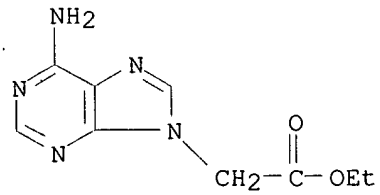
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New sub-monomer synthetic methods for the prepn. of peptide nucleic acid oligomeric structures are disclosed that provide for the synthesis of both predefined sequence peptide nucleic acid oligomers as well as random sequence peptide nucleic acid oligomers. Further these methods also provide for the incorporation of peptide nucleic acid units or strings of such units with amino acids or strings of amino acids in chimeric peptide nucleic acid-amino acid compds. Further disclosed are methods of making random libraries of peptide nucleic acids using the fully preformed monomers. Thus, a combinatorial library of chimeric peptide nucleic acid oligomers was prepd. using protected 2-oxomorphilone building blocks I-IV, which involved coupling of IV to a MBHA resin, Mitsunobu reaction of the resulting resin-bound hydroxy adduct with (Boc)2NH using Ph3P and di-Et azodicarboxylate, random coupling of the resulting resin-bound peptide nucleic acid monomer with a mixt. of I, II, III, and IV followed by Mitsunobu reaction for converting the terminal hydroxy group to the terminal amine moieties, repeating the latter procedure for extension of backbone and addn. of further nucleoside bases to complete the oligomer of the desired length, addn. of a peptide to the peptide nucleic acid unit using std. solid phase Merrifield peptide synthesis, and cleavage of peptide nucleic acid oligomers from the resin.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(improved prepn. of oligomeric peptide nucleic acid (PNA) combinatorial libraries)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



Searched by: Mary Hale 308-4258 CM-1 12D16

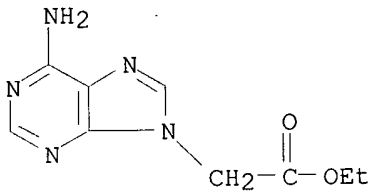
L27 ANSWER 29 OF 116 CAPLUS COPYRIGHT 2002 ACS
1998:589540 Document No. 129:276358 Preparation of nucleic acid-binding peptides using specific protection/deprotection strategy. Baetz, Hans Georg; Hansen, Henrik Frydenlund; Oerum, Henrik; Koch, Troels; Kofeod, Thomas (Boehringer Mannheim G.m.b.H., Germany). Jpn. Kokai Tokkyo Koho JP 10231290 A2 19980902 Heisei, 25 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-25937 19980206. PRIORITY: EP 1997-102028 19970208.

AB Title peptides are prepd. by (1) prepg. protected compds. having (a) plural ligands, which are bound to backbone, can be linked to bases of nucleic acids via H bond, and have primary or secondary amino group protected by strong-base-removable group and (b) backbones having NX1X2 (X1 = H, C1-3 alkyl, strong-acid-removable protecting group; X2 = strong-acid-removable protecting group), (2) removing the strong-acid-removable groups, and (3) removing the strong-base-removable groups. Two kinds of markers may be bound to the 2 kinds of deprotected amino groups. Monomers for the peptides are also claimed. The peptides are rapidly prepd. in high yield and large scale. The process is useful for prepn. of chimera compds. and S-S bond-contg. compds.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of nucleic acid-binding peptides using specific protection/deprotection strategy)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 30 OF 116 CAPLUS COPYRIGHT 2002 ACS
1998:504761 Document No. 129:250502 Molecular recognition of nucleolipid amphiphile octadecanoyl ester of 1-(2-carboxyethyl) adenine to the complementary nucleobases. Part I: characterization of the monolayer behavior at the air/water interface and photodimerization in the Langmuir-Blodgett film matrix under ultraviolet irradiation. Huang, Jianguo; Liang, Yingqiu (State Key Laboratory of Coordination Chemistry, Department of Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China). Thin Solid Films, 326(1,2), 217-222 (English) 1998. CODEN: THSFAP. ISSN: 0040-6090. Publisher: Elsevier Science S.A..

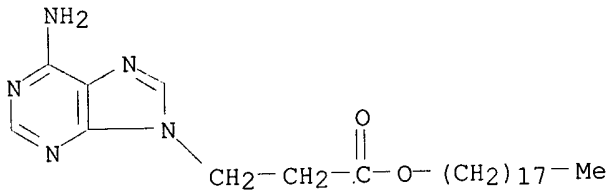
AB Mol. recognition capabilities of a novel nucleolipid amphiphile, octadecanoyl ester of 1-(2 carboxyethyl) adenine, to the complementary nucleobases at the air/water interface were investigated by surface pressure-area (.pi.-A) isotherms and UV spectra measurements. All of the observations show that mol. recognition through complementary base pairing takes place at the air/water interface between the adenine moiety in the headgroup of the nucleolipid amphiphile and the dissolved complementary nucleobase substrates in the subphase. On the surface of pure water, the monolayer gave a limiting mol. area of 29.3 .ANG.2 and collapse pressure at .apprxeq.62 mN/m while on the subphase of aq. 5 mM thymidine and uridine soln., the limiting mol. area and collapse pressure are 42.0 .ANG.2 and 77 mN/m, 39.7 .ANG.2 and 79 mN/m, resp. In the Langmuir-Blodgett (LB) matrix, the constituent mols. are arranged regularly, which facilitates the photodimerization of the thymine moieties and uracil moieties that transferred into solid substrates along with the surface monolayer of the nucleolipid amphiphile as a result of the

formation of the base-base complex, the photodimerization accomplished in 6 and 4 h for the thymine and uracil rings in the LB films under irradn. of a 254-nm UV light at room temp., resp.

IT **188524-32-5**, 9H-Purine-9-propanoic acid, 6-amino-, octadecyl ester
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(complementary nucleolipid; mol. recognition of nucleobases in aq. subphases of monolayers of)

RN 188524-32-5 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino-, octadecyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 31 OF 116 CAPLUS COPYRIGHT 2002 ACS

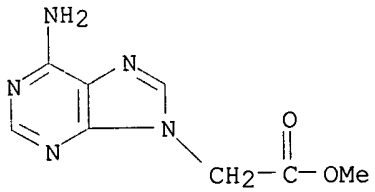
1998:464191 Document No. 129:216894 Solid-phase synthesis of peptide nucleic acid (PNA) monomers and their oligomerization using disulfide anchoring linkers. Aldrian-Herrada, Gudrun; Rabie, Alain; Wintersteiger, Reinhold; Brugidou, Jean (Karl-Franzens-Universitat, Graz, Austria). J. Pept. Sci., 4(4), 266-281 (English) 1998. CODEN: JPSIEI. ISSN: 1075-2617. Publisher: John Wiley & Sons Ltd..

AB A new simple solid-phase method has been developed for synthesizing Boc-protected peptide nucleic acid (PNA) monomers. An immobilized backbone was built on Expansin resin using an ester disulfide handle: 2-hydroxypropyl-dithio-2'-isobutyric acid (HPDI). The base acetic acids of thymine, Z-cytosine, Z-adenine, and 6-O-benzyl guanine were prepd. and coupled to the immobilized backbone. The HPDI handle was cleaved under mild conditions by cyanolysis or assisted hydrolysis with tris(2-carboxyethyl)phosphine (TCEP) to give undamaged PNA monomers. These monomers were coupled to form oligomers by the solid-phase method with another disulfide linkage: aminoethyldithio-2-isobutyric acid (AEDI) grafted on an amino-functionalized TentaGel resin, using in situ neutralization and TBTU as activating reagent. Final cleavage of the AEDI linker gave PNA bearing a cysteamide residue that could be useful for optimizing PNA properties. Oligomers of up to 16 residues long were assembled.

IT **23124-10-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of peptide nucleic acid monomers and their oligomerization using disulfide anchoring linkers)

RN 23124-10-9 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, methyl ester (8CI, 9CI) (CA INDEX NAME)



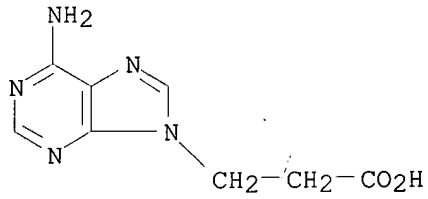
Searched by: Mary Hale 308-4258 CM-1 12D16

L27 ANSWER 32 OF 116 CAPLUS COPYRIGHT 2002 ACS
1998:451177 Document No. 129:189600 Base-specific interaction of polymers containing adenine: effect of chiral spacer on the interaction with polynucleotide. Inaki, Yoshiaki; Kamo, Shigeki; Miyata, Mikiji (Department of Materials and Life Science, Osaka University, Suita, 565, Japan). React. Funct. Polym., 37(1-3), 189-198 (English) 1998. CODEN: RFPOF6. ISSN: 1381-5148. Publisher: Elsevier Science B.V..

AB Polyethyleneimine derivs. of adenine with L- and D-serine as spacers were prepd. The polymer having D-serine spacer gave a stable polymer complex with poly(uridylic acid) (poly U), but the polymer having L-serine spacer gave an unstable polymer complex. The reason was concluded to be caused by the steric repulsion of L-serine units along the polymer chain when the polymer formed polymer complex with poly U.

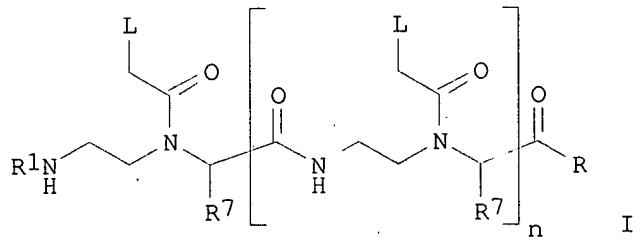
IT **4244-47-7**
RL: RCT (Reactant)
(base-specific interaction of polymers contg. adenine and the effect of chiral spacer on the interaction with polynucleotide)

RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 33 OF 116 CAPLUS COPYRIGHT 2002 ACS
1998:441926 Document No. 129:122864 Preparation of peptide nucleic acids having enhanced binding affinity and sequence specificity. Burchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik; Burchardt, Dorte (Isis Pharmaceuticals, Inc., Den.). U.S. US 5766855 A 19980616, 72 pp. Cont.-in-part of U. S. Ser. No. 108,591. (English). CODEN: USXXAM. APPLICATION: US 1996-686113 19960724. PRIORITY: DK 1991-986 19910524; DK 1991-987 19910524; DK 1992-510 19920415; US 1993-108591 19931122.

GI



I

AB A novel peptide nucleic acids I [each L = naturally occurring and non-naturally occurring nucleobase, with the proviso that at least one L = 2,6-diaminopurine; each R7 = H, C1-8 alkylamine; R = OH, NH2, NH-Lys-NH2; R1 = H, Ac, Me3CO2C (Boc); n = 1-30] bind complementary DNA and RNA

Searched by: Mary Hale 308-4258 CM-1 12D16

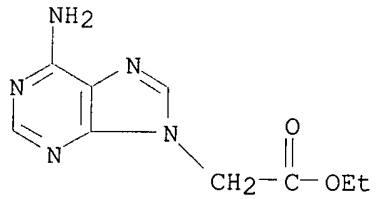
strands more strongly than a corresponding DNA strand, and exhibit increased sequence specificity and binding affinity. Methods of increasing binding affinity and sequence specificity of peptide nucleic acids are provided wherein some peptide nucleic acids comprise ligands selected from a group consisting of naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone, while other peptide nucleic acids contain at least one 2,6-diaminopurine nucleobase and at least one C1 -C8 alkylamine side chain. A variety of peptide nucleic acid contg. 2,6-diaminopurine and alkylamine side chains were prepd. and exhibited enhanced sequence selectivity and binding affinities with complementary DNA and RNA strands.

IT **25477-96-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of peptide nucleic acids having enhanced binding affinity and sequence specificity)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)

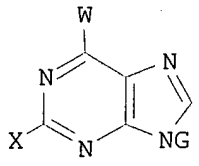


L27 ANSWER 34 OF 116 CAPLUS COPYRIGHT 2002 ACS

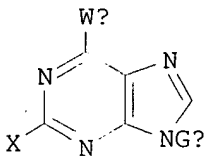
1998:430167 Document No. 129:95606 Procedure for the production of substituted purine derivatives, the agents containing them and their use as medicaments. Peyman, Anuschirwan; Knolle, Jochen; Wehner, Volkmar; Breipohl, Gerhard; Gourvest, Jean-Francois; Carniato, Denis; Gadek, Thomas Richard (Hoechst A.-G., Germany; Genentech Inc.). Ger. Offen. DE 19653646 A1 19980625, 32 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1996-19653646 19961220.

GI

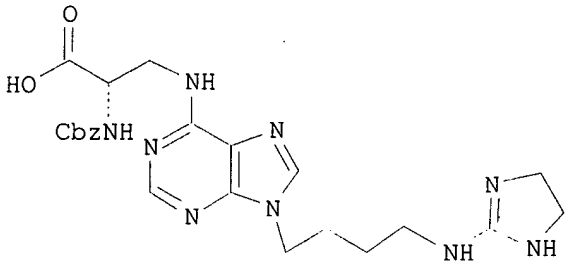
Searched by: Mary Hale 308-4258 CM-1 12D16



I



II



III

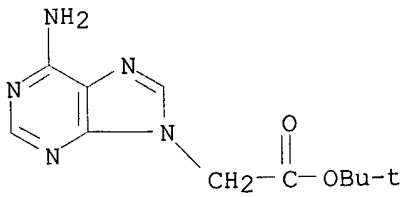
AB Purine derivs. I [G = (CR1R2)nA(CR1R2)m(CR1R3)i(CR1R2)q; W = B(CR1R2)rA1(CR1R2)s(CR1R3)k(CR1R2)tDE; X = H, NH2, NHCOR6; A, A1 = bond, CONR5, NR5CO, CO, NR5, O, S, SO, SO2, arylene, alkynylene, alkenylene; R1, R2 = H, F, Cl, CN, NO2, alkyl, cycloalkyl, (cycloalkyl)alkyl, aryl, arylalkyl, R6OR7, R6S(O)pR7, (R6)2NR7; R3 = H, F, Cl, CN, NO2, alkyl, cycloalkyl, (cycloalkyl)alkyl, aryl, arylalkyl, R6OR7, R6S(O)pR7, (R6)2NR7, R6CO2R7, R6COR7, R6OC(:O)R7, R6N(R5)CO2R7, R6S(O)pN(R5)R7, R6S(O)pN(R5)R7, R6S(O)pR7, R6SC(:O)N(R6)R7, R6COR6, R6N(R5)COR7, R6COR6, R6N(R5)COR7,R6N(R5)S(O)pR7; R4 = COR8, CSR8, S(O)pNR8, PO(R8)2, D-, L-amino acid; R5 = H, alkyl, cycloalkyl,(cycloalkyl)alkyl, aryl, arylalkyl; R6 = H, alkyl, cycloalkyl, (cycloalkyl)alkyl, aryl; R7 = bond, alkenylene; R8 = OH, alkoxy, arylalkoxy, aryloxy, (alkylcarbonyloxy)alkoxy, aryl(alkylcarbonyloxy)alkoxy, N(R6)2, (dialkylaminocarbonyl)methoxy, aryl(dialkylaminocarbonyl)methoxy, arylamino, L-, D-amino acid; B = O, S, NR5, NR5CO, CONR5, bond; D = bond, NR6, CONR6, NR6CO, SO2NR6, NR6CONR6, NR6CSNR6, NR6S(O)uNR6; E = H; m, n, s, t = 0 - 5; i, k = 0, 1; p, q = 0 - 2; r = 0 - 6; u = 1, 2] and. II [Ga = (CR1R2)rA1(CR1R2)s(CR1R3)k(CR1R2)tDE; Wa = B(CR1R2)nA(CR1R2)m(CR1R3)i(CR1R2)q] are useful as medicaments for treatment of osteoclastoma and retinopathy and as antiinflammation inhibitors, antitumor and cardiovascular agents. Thus, III was prepd. from 6-chloropurine via N9-alkylation with 4-MeC6H4SO3(CH2)4NHCO2CMe3, amination with H2NCH2CH(NHCbz)CO2H, and reaction with 2-(methylmercapto)-2-imidazoline hydroiodide. III showed antagonistic activity towards vitronectin receptor (.alpha..gamma..beta.3): IC50 = 0.075 .mu.M (95% inhibition at 10.mu.M).

IT **152774-16-8P**, N9-[(tert-Butoxycarbonyl)methyl]adenine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of substituted purines as vitronectin receptor antagonists)

RN 152774-16-8 CAPLUS

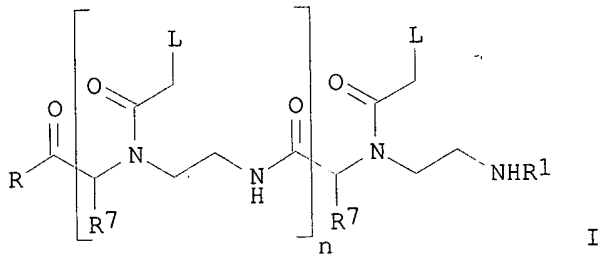
CN 9H-Purine-9-acetic acid, 6-amino-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16



L27 ANSWER 35 OF 116 CAPLUS COPYRIGHT 2002 ACS
1998:241026 Correction of: 1998:115390 Document No. 128:244346 Correction of: 128:177410 Preparation of peptide nucleic acids having enhanced binding affinity, sequence specificity and solubility. Buchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik (Den.). U.S. US 5714331 A 19980203, 68 pp. Cont.-in-part of U.S. Ser. No. 108,591. (English). CODEN: USXXAM. APPLICATION: US 1996-686116 19960724. PRIORITY: DK 1991-986 19910524; DK 1991-987 19910524; DK 1992-510 19920415; US 1993-108591 19931122.

GI

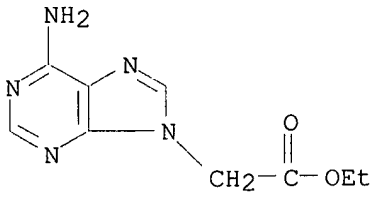


I

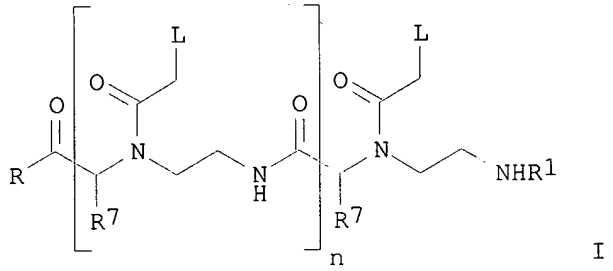
AB A novel class of compds., known as peptide nucleic acids (PNAs), e.g. I [each L = independently naturally occurring or non-naturally occurring nucleobase; each R7 = independently H, C1-7 alkylamine, with the proviso that at least one R7 = C1-7 alkylamine; R = OH, NH2, Lys-NH2; R1 = H, Ac, CO2CMe3 (Boc); n = 1-30], bind complementary DNA and RNA strands more strongly than a corresponding DNA strand, and exhibit increased sequence specificity and soly. The peptide nucleic acids comprise ligands selected from a group consisting of naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone, and contain alkylamine side chains. Thus, the Tm for PNA H-GTkAGATkCACTk-NH2 (II; aminoethylglycine backbone except where k appears, which is aminoethyl-D-lysine) binding to antiparallel complementary DNA was 55.degree. while that for for PNA H-GTAGATCACT-NH2 (III; with aminoethylglycine backbone) was 52.degree.. The presence of the D-Lys also enhanced sequence specificity: in the presence of a single mismatch in the complementary DNA, the Tm's were 38.degree. and 42.degree. for II and III, resp. A 16-mer PNA contg. four lysine side chains was sol. in physiol. useful solns. while the PNA devoid of the lysine side chains was insol. A 12-mer PNA contg. two 2,6-diaminopurine nucleobases bearing Lys side chains, prepd. by solid-phase methods using N.alpha.-Boc and benzyl side chain protection, blocked in vitro translation of hepatitis C virus protein with EC50 = 29 nM.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of peptide nucleic acids having enhanced binding affinity,

sequence specificity and soly.)
RN 25477-96-7 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)

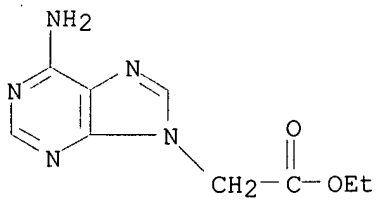


L27 ANSWER 36 OF 116 CAPLUS COPYRIGHT 2002 ACS
1998:146586 Document No. 128:192941 Preparation of peptide nucleic acids having enhanced binding affinity, sequence specificity and solubility. Buchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik (Den.). U.S. US 5719262 A 19980217, 70 pp. Cont.-in-part of U.S. Ser. No. 108,591. (English). CODEN: USXXAM. APPLICATION: US 1996-685484 19960724. PRIORITY: US 1993-108591 19931122.
GI

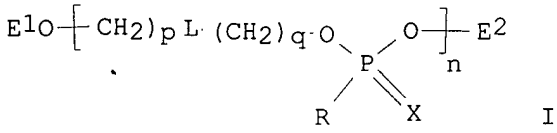


AB A novel class of compds., known as peptide nucleic acids (PNAs), e.g. I [each L = independently naturally occurring or non-naturally occurring nucleobase; each R7 = independently H, C1-7 alkylamine, with the proviso that at least one R7 = C1-7 alkylamine; R = OH, NH2, Lys-NH2; R1 = H, Ac, CO2CMe3 (Boc); n = 1-30], bind complementary DNA and RNA strands more strongly than a corresponding DNA strand, and exhibit increased sequence specificity and soly. The peptide nucleic acids comprise ligands selected from a group consisting of naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone, and contain alkylamine side chains. Thus, a 12-mer PNA contg. two 2,6-diaminopurine nucleobases bearing Lys sidechains, prepd. by solid-phase methods using N.alpha.-Boc and benzyl side chain protection, blocked in vitro translation of hepatitis C virus protein with EC50 = 29 nM.
IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of peptide nucleic acids having enhanced binding affinity, sequence specificity and soly.)
RN 25477-96-7 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

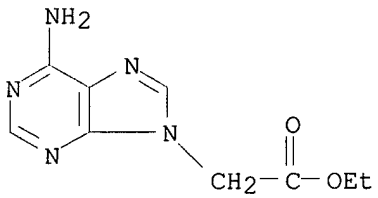


L27 ANSWER 37 OF 116 CAPLUS COPYRIGHT 2002 ACS
1998:118624 Document No. 128:167656 Combinatorial library on the preparation of oligodeoxyribonucleotide phosphoramidates and phosphorothiomidates as phospholipase A2 inhibitors. Cook, Phillip Dan; Acevedo, Oscar; Hebert, Normand (ISIS Pharmaceuticals, Inc., USA). U.S. US 5717083 A 19980210, 26 pp. Cont.-in-part of U.S. 5,637,684. (English). CODEN: USXXAM. APPLICATION: US 1996-693112 19960819. PRIORITY: US 1994-200638 19940223; WO 1995-US2267 19950223.
GI



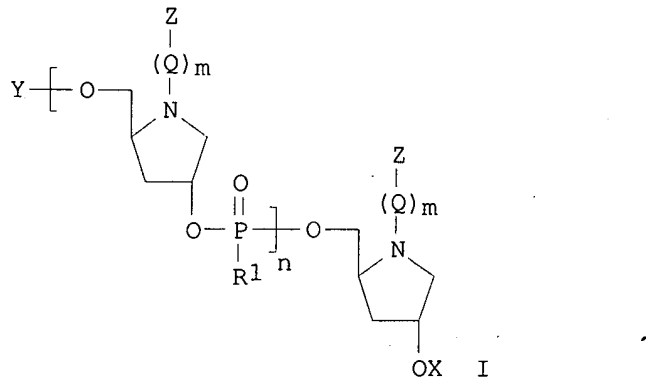
I

AB Combinatorial library on the prepn. of title oligodeoxyribonucleotides I (X = O, S; R = amine, N-contg. heterocycle; L = alkyl, alkenyl, alkynyl, carbocycle, heterocycle; E1, E2 = independently H, hydroxyl protecting group, activated solid support; p, q = 0-6; n = 2-50) were prepd. as phospholipase A2 inhibitors.
IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (combinatorial library on the prepn. of oligodeoxyribonucleotide phosphoramidates and phosphorothiomidates as phospholipase A2 inhibitors)
RN 25477-96-7 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 38 OF 116 CAPLUS COPYRIGHT 2002 ACS
1998:98080 Document No. 128:167655 Combinatorial library on the preparation of pyrrolidine-containing monomers and oligomers as phospholipase A2 inhibitors and anti-inflammatory agents. Acevedo, Oscar L.; Hebert, Normand (ISIS Pharmaceuticals, Inc., USA). U.S. US 5714606 A 19980203, 30 pp. Cont.-in-part of U.S. 5,519,134. (English). CODEN: USXXAM. APPLICATION: US 1996-669505 19960815. PRIORITY: US 1994-180134 19940111; WO 1995-US356 19950111.
GI

Searched by: Mary Hale 308-4258 CM-1 12D16

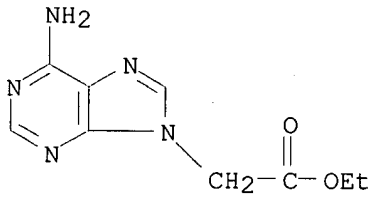


AB Combinatorial library on the prepn. of pyrrolidine-contg. monomers and oligomers I [X = H, phosphate, activated phosphate group, phosphite, solid support, oligonucleotide; Y = H, hydroxyl protecting group, conjugate group, oligonucleotide; R1 = OH, SH; Z = alkyl, alkenyl, alkynyl, aryl, alkoxy, thioalkyl, amino, imine, CHO, ester, nitrogen-contg. heterocycle, purine, pyrimidine, phosphate, polyether group, polyethylene glycol group, metal coordination group; Q = alkyl, acyl, C(O)-O, C(O)-NH, C(S)-O, C(S)-NH, SO2; n = 1-50; m = 0-1] is reported. Thus, I [X = P(OCH2CH2CN)NPri2; Z = CH2PH; Q = CO; m = 1; n = 0; Y = dimethoxytrityl] was prepd. as inhibitors of phospholipase A2 and used for the treatment of inflammatory diseases including atopic dermatitis and inflammatory bowel disease.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (combinatorial library on prepn. of pyrrolidine-contg. monomers and oligomers as phospholipase A2 inhibitors and anti-inflammatory agents)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)

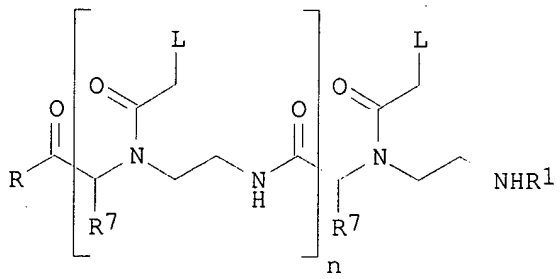


L27 ANSWER 39 OF 116 CAPLUS COPYRIGHT 2002 ACS

1998:89263 Document No. 128:180668 Preparation of peptide nucleic acids having enhanced binding affinity, sequence specificity and solubility. Nielsen, Peter E.; Egholm, Michael; Berg, Rolf H. (Buchardt, Dorte, Den.; Isis Pharmaceuticals, Inc.; Nielsen, Peter E.; Egholm, Michael; Berg, Rolf H.). PCT Int. Appl. WO 9803542 A1 19980129, 150 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, US, US, US, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH,

CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US12811 19970724. PRIORITY: US 1996-685484 19960724; US 1996-686116 19960724; US 1996-686114 19960724; US 1996-686113 19960724; US 1997-51002 19970529.

GI



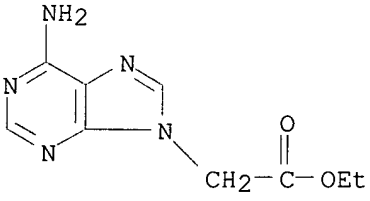
I

AB A novel class of compds., known as peptide nucleic acids (PNAs), e.g. I [each L = independently naturally occurring or non-naturally occurring nucleobase; each R7 = independently H, C1-7 alkylamine, with the proviso that at least one R7 = C1-7 alkylamine; R = OH, NH2, Lys-NH2; R1 = H, Ac, CO2CMe3 (Boc); n = 1-30], bind complementary DNA and RNA strands more strongly than a corresponding DNA strand, and exhibit increased sequence specificity and soly. The peptide nucleic acids comprise ligands selected from a group consisting of naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone, and contain C1-C8 alkylamine side chains. Methods of enhancing the soly., binding affinity and sequence specificity of PNAs are provided. Thus, a 12-mer PNA contg. two 2,6-diaminopurine nucleobases bearing Lys sidechains, prepd. by solid-phase methods using N.alpha.-Boc and benzyl side chain protection, blocked in vitro translation of hepatitis C virus protein with EC50 = 29 nM.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of peptide nucleic acids having enhanced binding affinity, sequence specificity and soly.)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 40 OF 116 CAPLUS COPYRIGHT 2002 ACS

1998:50910 Document No. 128:154336 Oligonucleotide analogs with 4-hydroxy-N-acetylprolinol as sugar substitute. Ceulemans, Griet; Van Aerschot, Arthur; Wroblowski, Berthold; Rozenski, Jef; Hendrix, Chris; Herdewijn, Piet (Laboratory of Medicinal Chemistry, Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.). Chem.--Eur. J., 3(12), 1997-2010 (English) 1997. CODEN: CEUJED. ISSN: 0947-6539. OTHER SOURCES: CASREACT 128:154336. Publisher: Wiley-VCH

Searched by: Mary Hale 308-4258 CM-1 12D16

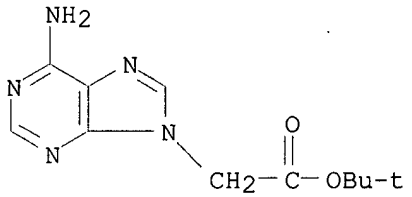
Verlag GmbH.

AB Modified oligonucleotides incorporating trans-4-hydroxy-N-acetyl-L-prolinol (trans-4-HO-L-NAP) or its D-analog as sugar substitute were synthesized with adenine and thymine as nucleobases. All-adenine oligonucleotides built from (2S,4S) or (2R,4R)-cis-4-hydroxy-N-acetylprolinol were likewise prepd. Hybridization studies revealed that hetero-complexes formed between polyU and homochiral trans-4-hydroxy-N-acetylprolinol-based oligomers of the same as well as of opposite chirality (polyU/trans-DA13* and polyU/trans-LA13*). The former, however, were triple-stranded. Other complexes with ribonucleic acids were polyA/trans-LT13* and polyU/cis-LA13*. Hetero-duplexes with deoxy-nucleic acids were formed between trans-LA13* and oligo-thymidylate. Interaction was also obsd. for cis-LA13* and oligo-thymidylate, but not with the D-hydroxyprolinol analogs. Microcalorimetry proved this interaction to be the formation of a triple-stranded complex. Two hetero-duplexes, trans-LA13*/dT13 and trans-LA13*/polyU, had similar or slightly increased stability when compared to the natural dA13/dT13 or dA13/polyU systems. Microcalorimetry clearly indicated the formation of a duplex, in contrast to interactions with N-acetylprolinol oligonucleotides of different stereochem. Moreover, the enthalpy change was of the same magnitude but the assocn. const. was slightly lower. Natural nucleic acids thus clearly prefer hybridization with L-hydroxyprolinol oligomers over D-hydroxyprolinol oligomers. For the series investigated, the L-trans oligomers seem best to mimic natural oligonucleotides. These modified oligonucleotides formed homo-complexes if both strands were of the same chirality, i.e., homo-complexes formed between trans-LA* and trans-LT* and between trans-DA* and trans-DT*, reflecting the iso-chiral pu-py pairing found in natural nucleic acids. Once more, however, calorimetry proved these to be triplex interactions. Hetero-chiral pairing was not obsd. between modified oligonucleotides, but only between modified oligonucleotides and natural polyU. The thermal stabilities of these hetero-chiral complexes differed clearly.

IT **152774-16-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(oligonucleotide analogs with 4-hydroxy-N-acetylprolinol as sugar substitute)

RN 152774-16-8 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 41 OF 116 CAPLUS COPYRIGHT 2002 ACS

1997:804926 Document No. 128:75666 Liquid phase synthesis of peptide nucleic acid (or polyamide nucleic acid) dimers. Farese, Audrey; Pairot, Sandrine; Patino, Nadia; Ravily, Veronique; Condom, Roger; Aumelas, Andre; Guedj, Roger (Laboratoire de Chimie Bio-Organique, CNRS ESA 6001, Universite de Nice Sophia-Antipolis, Nice, F-06108, Fr.). Nucleosides Nucleotides, 16(10 & 11), 1893-1906 (English) 1997. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Marcel Dekker, Inc..

AB The liq. phase synthesis of "polyamide nucleic acid" (PNA) dimers contg. the purine nucleic acid bases adenine and guanine has been achieved in good yields. This strategy was elaborated in order to circumvent

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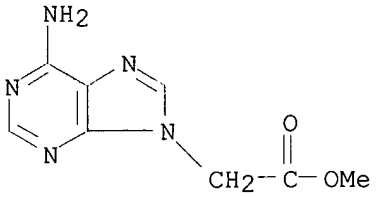
difficult direct coupling of protected PNA monomers. This method can be applied to the liq. phase synthesis of short protected polyPNAs fragments, which can then selectively be deprotected.

IT **23124-10-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(liq. phase synthesis of peptide nucleic acid dimers)

RN 23124-10-9 CAPLUS

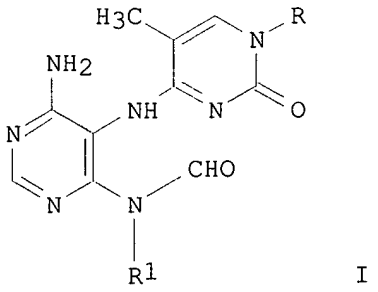
CN 9H-Purine-9-acetic acid, 6-amino-, methyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 42 OF 116 CAPLUS COPYRIGHT 2002 ACS

1997:724059 Document No. 127:346600 Photochemistry of 4-Thiothymine Derivatives in the Presence of N-9-Substituted-Adenine Derivatives: Formation of N-6-Formamidopyrimidines. Saintome, Carole; Clivio, Pascale; Favre, Alain; Fourrey, Jean-Louis (Institut de Chimie des Substances Naturelles, CNRS, Gif-sur-Yvette, 91198, Fr.). J. Org. Chem., 62(23), 8125-8130 (English) 1997. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

GI



I

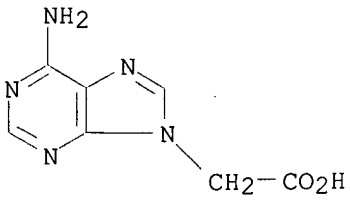
AB UV irradn. of aq. solns. contg. either 4-thiothymin-1-ylacetic acid (I) and adenosine (II), 4-thiothymidine (III) and adenin-9-ylacetic acid (IV), or I and IV led to 4,5-diamino-6-formamidopyrimidines, e.g. V (R = 2'-deoxyribofuranosyl, R1 = ribofuranosyl). These new observations demonstrate that the replacement of one or both nucleoside sugar residues by a carboxymethyl group does not affect the regioselective course of the photochem. reaction. The thermal decompn. of V that resulted from irradn. of III in the presence of II, was examd. along with its behavior under mild alk. conditions. This study is related to the mechanism of DNA damage caused by UV irradn. and formation of N-6-formamidopyrimidines.

IT **20128-29-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(photochem. of thiothymines in the presence of substituted-adenines and formation of formamidopyrimidines)

RN 20128-29-4 CAPLUS

Searched by: Mary Hale 308-4258 CM-1 12D16

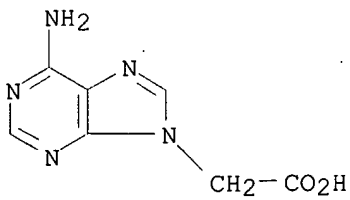
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 43 OF 116 CAPLUS COPYRIGHT 2002 ACS
1997:714365 Document No. 128:23092 Oligonucleotides with 3-hydroxy-N-acetylprolinol as sugar substitute. Ceulemans, Griet; Van Aerschot, Arthur; Rozenski, Jef; Herdewijn, Piet (Laboratory of Medicinal Chemistry, Rega Institute for Medical Research, K.U. Leuven, Louvain, B-3000, Belg.). Tetrahedron, 53(44), 14957-14974 (English) 1997. CODEN: TETRAB. ISSN: 0040-4020. Publisher: Elsevier.

AB Fully modified oligonucleotides were synthesized from the 3-O-phosphoramidites of monomethoxytritylated trans-3-hydroxy-N-[(N6-benzoyladenin-9-yl)-acetyl]-prolinol [(2S,3R) and (2R,3S) series], trans-3-hydroxy-N-[(thymin-1-yl)-acetyl]-prolinol [(2S,3R) and (2R,3S) series], and cis-3-hydroxy-N-[(N6-benzoyl-adenin-9-yl)-acetyl]-L-prolinol (2R,3R). Remarkably, as well the L-trans (2R,3S) as the D-trans (2S,3R) all-adenine oligonucleotides are capable of hybridization with complementary DNA and RNA. With modified all-thymine trans-oligomers no complexation with natural nucleic acids was obsd. However, complex formation between two modified strands of the same sense of chirality does occur with formation of a triple stranded complex. The all-thymine oligonucleotides with trans-3-HO-N-acetylprolinol backbone are capable of hybridization with trans-4-HO-N-acetylprolinol oligoadenylates of the same enantiomeric form in both the D and the L series, and inversely, the all-adenine oligonucleotide with the trans-3-HO conformation hybridizes with the trans-4-HO oligothymidylates. While the former interactions have a triple stranded origin, the latter are 1:1 interactions. No interactions were noticed upon mixing oligonucleotide analogs of different sense of chirality. Modified mixed trans-3-HO A,T sequences display no hybridization with complementary nucleic acids, nor homocomplex formation. The L-cis all-adenine oligonucleotide hybridizes with its RNA complement. Several complexes were investigated by CD and microcalorimetry. In conclusion, the 3-hydroxy-N-acetylprolinol system represents an example of homochiral oligonucleotides built up from two enantiomeric forms and hybridizing both with natural nucleic acids.

IT **20128-29-4**
RL: RCT (Reactant)
(oligonucleotides with hydroxyacetylprolinol as sugar substitute)
RN 20128-29-4 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



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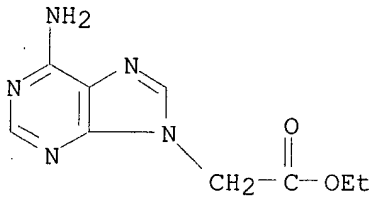
L27 ANSWER 44 OF 116 CAPLUS COPYRIGHT 2002 ACS
1997:580887 Document No. 127:262956 Synthesis and biochemical properties of phosphonyl acyclic analogs of 2'-deoxyadenosine nucleotides. Malakhov, D. V.; Semizarov, D. G.; Yas'ko, M. V. (Engelhardt Inst. Mol. BIol., Russ. Acad. Sci., Moscow, 117984, Russia). Bioorg. Khim., 21(7), 539-544 (Russian) 1995. CODEN: BIKHD7. ISSN: 0132-3423. Publisher: MAIK Nauka.

AB 9-[2-(Phosphonomethylcarbonylamino)ethyl]adenine, 9-[(2-phosphonoethyl)aminocarbonylmethyl]adenine, 9-{2-[(2-phosphonoethyl)carbonylamino]ethyl}adenine and their diphosphates were synthesized. All three diphosphates were shown to incorporate into the 3'-terminus of the DNA chain during the synthesis of the avian myeloblastose virus catalyzed by reverse transcriptase. However, they do not serve as substrates for DNA polymerase .alpha. from human placenta, polymerase .beta. from calf thymus, or terminal deoxynucleotidyl transferase from calf thymus.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and biochem. properties of phosphonyl acyclic analogs of deoxyadenosine nucleotides)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 45 OF 116 CAPLUS COPYRIGHT 2002 ACS
1997:526712 Document No. 127:191025 Synthesis and Activity of 6-Substituted Purine Linker Amino Acid Immunostimulants. Zacharie, Boulos; Gagnon, Lyne; Attardo, Giorgio; Connolly, Timothy P.; St-Denis, Yves; Penney, Christopher L. (Department of Medicinal Chemistry, BioChem Therapeutic Inc., Laval, PQ, H7V 4A7, Can.). J. Med. Chem., 40(18), 2883-2894 (English) 1997. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

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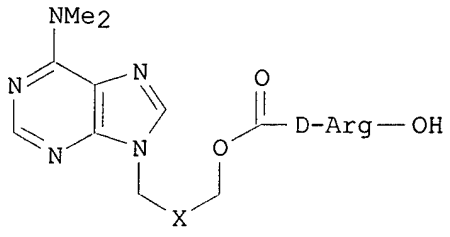

I

AB A series of 6-substituted purinyl alkoxycarbonyl amino acids, e.g. I (X = divalent linker group) were synthesized and evaluated for their ability to stimulate cytotoxic T lymphocytes (CTLs) and the mixed lymphocyte reaction (MLR). A few of these compds., in particular I [X = (CH2)3] (BCH-1393), displayed an in vitro stimulation of CTLs comparable to interleukin 2 (IL

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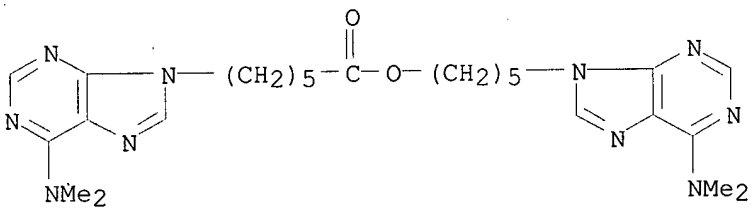
2). BCH-1393 increased the CTL response between 10-9 M and 10-5 M. Further, this potent in vitro activity was reflected as a significant increase in CTL cell no. in vivo. However, immunophenotyping of some of the other equipotent compds. did not reveal a parallel relative increase in CTLs in vivo. It was difficult to formulate a rigorous structure-activity relationship based on in vitro CTL activity. Nevertheless, the activity was dependent upon the nature of the 6-substituent on the purine, the type and stereochem. of the amino acid, and the distance and spatial freedom between the purine and amino acid as defined by the length and rigidity of the linker. These compds. were generally nontoxic, as exemplified by BCH-1393. BCH-1393 is a promising immunostimulant which may be targeted for those disease states which require an increased CTL or TH1 type response.

IT **194225-62-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and activity of substituted purine linker amino acid immunostimulants)

RN 194225-62-2 CAPLUS

CN 9H-Purine-9-hexanoic acid, 6-(dimethylamino)-, 5-[6-(dimethylamino)-9H-purin-9-yl]pentyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 46 OF 116 CAPLUS COPYRIGHT 2002 ACS

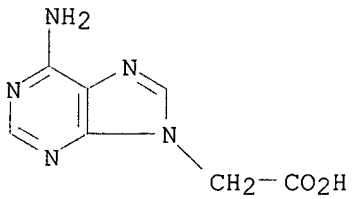
1997:193437 Document No. 126:271759 Pharmacokinetics and metabolism of selected prodrugs of PMEA in rats. Shaw, Jeng-Pyng; Louie, Michael S.; Krishnamurthy, V. V.; Arimilli, Murty N.; Jones, Robert J.; Bidgood, Alison M.; Lee, William A.; Cundy, Kenneth C. (Gilead Sciences, Inc., Foster City, CA, 94404, USA). Drug Metab. Dispos., 25(3), 362-366 (English) 1997. CODEN: DMDSAI. ISSN: 0090-9556. Publisher: Williams & Wilkins.

AB The oral bioavailability of PMEA (9-[2-(phosphonomethoxy)ethyl]adenine; adefovir) has been detd. in rats from three bis-ester prodrugs of PMEA: bis-(pivaloyloxymethyl) PMEA (bis-POM PMEA), bis-(phenyl) PMEA, and bis-(o-ethoxyphenyl) PMEA. The prodrugs were each administered to 9 male rats as solns. in PEG 400 at a dose of 10 mg-equiv. of PMEA per kg. Plasma samples were obtained over the course of 12 h and concns. of PMEA were detd. by fluorescence derivatization and anal. by HPLC. Concns. of PMEA obsd. in plasma following oral administration of PMEA prodrugs were compared with levels obsd. for i.v. PMEA. The obsd. oral bioavailabilities of PMEA from bis-POM PMEA, bis-(phenyl) PMEA, and bis-(o-ethoxyphenyl) PMEA were 38.2%, 2.46%, and 40.1%, resp. PMEA was the only metabolite formed after oral administration of bis-POM PMEA. Three metabolites were detected after oral administration of either bis-(phenyl) PMEA or bis-(o-ethoxyphenyl) PMEA to rats: PMEA, the corresponding monoester, and 2-adenylacetic acid. The major metabolite of bis-(phenyl) PMEA was 2-adenylacetic acid following oral administration. 2-Adenylacetic acid appears to have been formed from the intact prodrugs by a P 450 mediated oxidn. of the Et side chain.

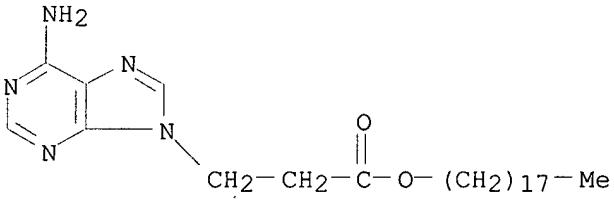
IT **20128-29-4**
RL: MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

Searched by: Mary Hale 308-4258 CM-1 12D16

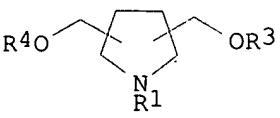
(pharmacokinetics and metab. of selected prodrugs of PMEA in rats)
RN 20128-29-4 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 47 OF 116 CAPLUS COPYRIGHT 2002 ACS
1997:130890 Document No. 126:238595 Synthesis of novel nucleolipid amphiphiles. Huang, Jianguo; Ding, Daoyuan; Zhang, Zhiqiang; Shi, Bo; Liang, Yingqiu (Dep. Chem., Coordination Chem. Inst. and State Key Lab. Coordination Chem., Nanjing Univ., Nanjing, 210093, Peop. Rep. China). Synth. Commun., 27(4), 681-690 (English) 1997. CODEN: SYNCAV. ISSN: 0039-7911. Publisher: Dekker.
AB Three derivs. of uridine, thymidine and adenosine with one or two stearoyl chains, and three kinds of lipids with one or two nucleic acid bases were synthesized, which can form a stable monolayer at the air-water interface.
IT **188524-32-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of nucleolipid amphiphiles)
RN 188524-32-5 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino-, octadecyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 48 OF 116 CAPLUS COPYRIGHT 2002 ACS
1997:127453 Document No. 126:144106 Combinatorial libraries having aminodiol monomer subunits. Hebert, Normandy (Isis Pharmaceuticals, Inc., USA; Hebert, Normandy). PCT Int. Appl. WO 9640672 A1 19961219, 174 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US9604 19960607. PRIORITY: US 1995-483311 19950607.
GI



I

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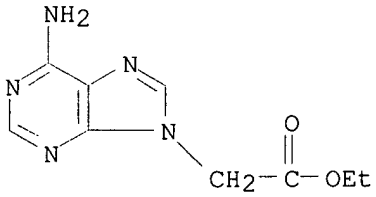
AB Combinatorial libraries constructed to include aminodiol monomer subunits connected by phosphodiester, phosphorothioate, or phosphoramidate linking moieties were described. Thus, oligomeric compds. and libraries of such compds. comprising a plurality of aminodiol monomer subunits, e.g., I [R1 = TL or a protective group; L = (cyclo)alk(en)yl, aryl, heterocyclyl, etc.; R3,R4 = H, protective group, P(O)R, etc.; R = OH, (di)alkylamino, etc.; T = bond, CH2, {[CR6R7]mR5[CR8R9]n[CR10]pE}q(sic); E,R5 = bond, CH:CH, C.tplbond.C, O, NR11, etc.; R10 = O, S, NR11; R6-R9,R11 = H, (halo)alkyl, aryl, etc.; m,n = 0-5; p = 0 or 1; q = 1 to about 10 (sic)] joined by linking groups were claimed.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(combinatorial libraries having aminodiol monomer subunits)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 49 OF 116 CAPLUS COPYRIGHT 2002 ACS

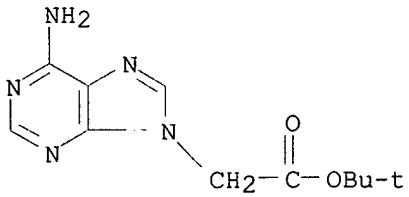
1997:119217 Document No. 126:131753 PNA-DNA chimeras and PNA synthons for their preparation. Gildea, Brian D.; Coull, James M. (Perseptive Biosystems, Inc., USA). PCT Int. Appl. WO 9640709 A1 19961219, 99 pp. DESIGNATED STATES: W: JP; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US7844 19960529. PRIORITY: US 1995-480228 19950607.

AB A method is disclosed for the prepn. of novel peptide nucleic acid (PNA) synthons compatible with DNA synthetic reagents and instrumentation. Accordingly, the PNA synthons of this invention are particularly suitable for the prepn. of PNA-DNA chimeras, among other oligomers. The PNA synthons are designed to have a protecting group strategy which is orthogonal and allows removal of the protecting groups under mild conditions. Generally, an acid labile protected backbone is coupled to a nucleobase side chain moiety to form the PNA synthon. A novel method for synthesizing the acid labile protected backbone also is described. In addn., novel compns. of matter are disclosed.

IT **152774-16-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(peptide nucleic acid-DNA chimeras and PNA synthons for their prepn.)

RN 152774-16-8 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

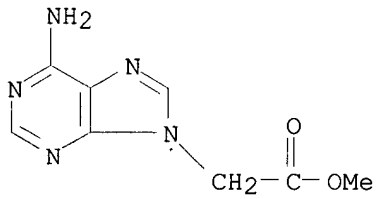


Searched by: Mary Hale 308-4258 CM-1 12D16

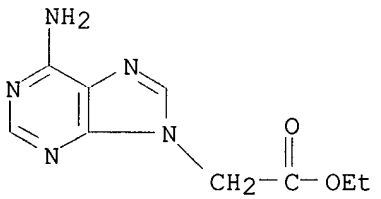
L27 ANSWER 50 OF 116 CAPLUS COPYRIGHT 2002 ACS
1997:111176 Document No. 126:118200 Improved synthons for the synthesis and deprotection of peptide nucleic acids under mild conditions. Coull, James M.; Egholm, Michael; Hodge, Richard P.; Ismail, Mohamed; Rajur, S. B. (Perseptive Biosystems, Inc., USA). PCT Int. Appl. WO 9640685 A1 19961219, 138 pp. DESIGNATED STATES: W: JP; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US9144 19960606. PRIORITY: US 1995-487666 19950607.

AB A method is disclosed for prepg. novel peptide nucleic acid (PNA) synthons having protecting groups capable of removal under mild conditions. The PNA synthons are prepd. by coupling novel N-substituted nucleobase intermediates having a carbamate protection of the exocyclic amino group of the heterocycle to an amino protected backbone or an amino protected backbone ester of the amino acid N-(2-aminoethyl)glycine. The resultant PNA synthons have orthogonal protection of the carbamate protected nucleobase and the amino protected backbone. Thus, a soln. of N6-(benzhydryloxycarbonyl)-9-adenylacetic acid (QOH) in MeCN contg. N-methylmorpholine and pivaloyl chloride was combined with a suspension of FmocNHCH2CH2NRCH2CO2H (I; Fmoc = fluorenylmethoxycarbonyl, R = H) in MeCN-H2O contg. Et3N to afford 87.5% I (R = Q).

IT **23124-10-9**
RL: RCT (Reactant)
(prepn. of synthons for synthesis and deprotection of peptide nucleic acid)
RN 23124-10-9 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, methyl ester (8CI, 9CI) (CA INDEX NAME)



IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of synthons for synthesis and deprotection of peptide nucleic acid)
RN 25477-96-7 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 51 OF 116 CAPLUS COPYRIGHT 2002 ACS
1996:728034 Document No. 126:60309 Thermodynamic effect of complementary hydrogen bond base pairing on aromatic stacking interaction in the guanine-X-Trp complex (X = adenine, guanine, cytosine, thymine). Tarui, Mariko; Nomoto, Noriko; Hasegawa, Yoko; Minoura, Katsuhiko; Doi,

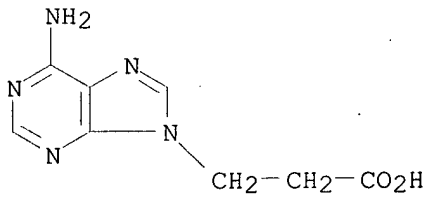
Mitsunobu; Ishida, Toshimasa (Dep. Physical Chem., Osaka Univ. Pharmaceutical Scis., Osaka, 569-11, Japan). Chem. Pharm. Bull., 44(11), 1998-2002 (English) 1996. CODEN: CPBTAL. ISSN: 0009-2363. Publisher: Pharmaceutical Society of Japan.

AB Four kinds of X-Trp-OH (X = adenine, guanine, cytosine, thymine) mols. were prepd. as model compds. to investigate the effect of complementary hydrogen bond base pairing on the stacking interaction of Trp with nucleic acid base. Assocn. consts. (Ka) of these compds. with two guanine derivs. (9-ethylguanine and 9-ethyl-7-methylguanine) were det. by Eadie-Hifstee plots of 1H-NMR titrn. expts., and the thermodn. parameters (.DELTA.H, .DELTA.S and .DELTA.G) for the resp. complexes were obtained by van't Hoff analyses based on the temp. dependence of the Ka values. The complexes were characterized by enthalpy/entropy compensations, where the interaction of cytosine-Trp with guanine derivs. was largely enthalpy-driven, accompanied by a small entropy component, whereas those of remaining complexes were all assocd. with a large increase in entropy, accompanied by a small pos. enthalpy component. The present insight on the binding of increase in entropy, accompanied by a small pos. enthalpy component. The present insight on the binding of X-Trp with a guanine base provides a thermodn. basis for the importance of cooperative hydrogen bond pairing and arom. stacking interactions in the specific recognition of a nucleic acid base pair by protein.

IT **4244-47-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(effect of complementary hydrogen bond and base pairing on arom. stacking in tryptophan-nucleic acid base conjugates)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 52 OF 116 CAPLUS COPYRIGHT 2002 ACS

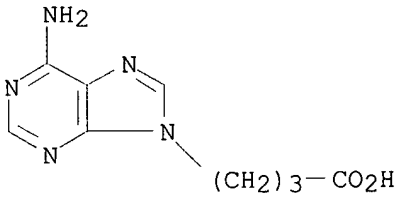
1996:644872 Document No. 126:7881 Synthesis and some spectroscopic properties of porphyrin derivatives connected with nucleobases (adenine, thymine, guanine and cytosine) by alkanamide chains. Hisatome, Masao; Maruyama, Noriaki; Ikeda, Koichi; Furutera, Tetsuo; Ishikawa, Tomiyasu; Yamakawa, Koji (Fac. Pharmaceutical Sciences, Science Univ. Tokyo, Tokyo, 162, Japan). Chem. Pharm. Bull., 44(10), 1801-1811 (English) 1996. CODEN: CPBTAL. ISSN: 0009-2363. Publisher: Pharmaceutical Society of Japan.

AB Several kinds of porphyrin derivs. covalently connected with adenine, thymine, guanine, cytosine or with the adenine-thymine pair in a stacking mode have been synthesized via amidation of (2-aminophenyl)porphyrin derivs. with nucleobase-alkanoic acids, and characterized by spectroscopic methods. In the 1H-NMR spectra of these nucleobase-porphyrins the proton signals of the nucleobase moieties appear at remarkably higher fields than those of the ref. compds. (the corresponding nucleobase-alkanoates) which have no porphyrin moiety. The behaviors of the high field shifts, due to the diamagnetic ring current effect of the porphyrin ring, reflect the characteristic conformational features of these compds. in which the base moieties are located at the upper zone of the porphyrin ring. The Soret bands of the porphyrin in the electronic absorption spectra were markedly weaker in intensity compared with those of the ref. compd. which has no

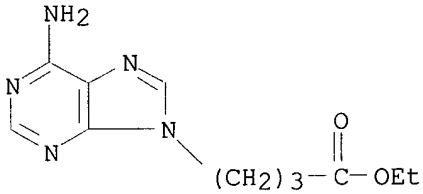
nucleobase moiety. Both the high-field shifts of the base protons and the hypochromic effects on the Soret band are larger in guanine and cytosine systems than those in adenine and thymine systems, resp. These results indicate a greater affinity of guanine and cytosine for porphyrin in comparison with adenine and cytosine, resp., and this conclusion is compatible with the reported electronic spectral properties of mixts. of polynucleotides and water-sol. porphyrin derivs.

IT **33147-28-3P 41785-06-2P 90973-36-7P 102788-98-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectroscopic properties of porphyrins covalently linked to nucleic acid bases)

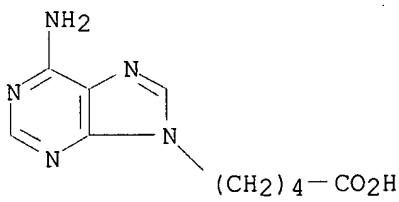
RN 33147-28-3 CAPLUS
CN 9H-Purine-9-butanoic acid, 6-amino- (9CI) (CA INDEX NAME)



RN 41785-06-2 CAPLUS
CN 9H-Purine-9-butanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)

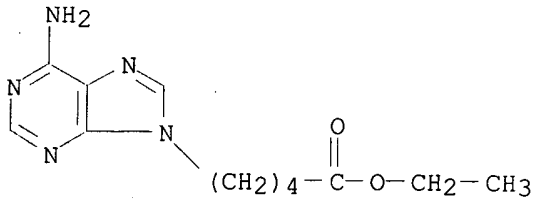


RN 90973-36-7 CAPLUS
CN 9H-Purine-9-pentanoic acid, 6-amino- (9CI) (CA INDEX NAME)



RN 102788-98-7 CAPLUS
CN 9H-Purine-9-pentanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)

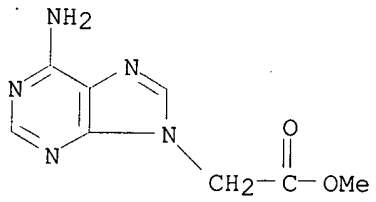
Searched by: Mary Hale 308-4258 CM-1 12D16



L27 ANSWER 53 OF 116 CAPLUS COPYRIGHT 2002 ACS
1996:585791 Document No. 125:320771 Synthesis and properties of DNA-PNA chimeric oligomers. Finn, Patrick J.; Gibson, Neil J.; Fallon, Rachel; Hamilton, Alan; Brown, Tom (Dep. Chemistry, Univ. Southampton, Highfield, Southampton, SO17 1BJ, UK). Nucleic Acids Res., 24(17), 3357-3363 (English) 1996. CODEN: NARHAD. ISSN: 0305-1048.

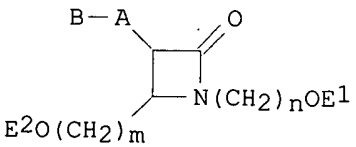
AB Adenine, thymine and cytosine PNA (peptide nucleic acid) monomers have been prepd. using 3-amino-1,2-propanediol as a starting material. The benzoyl group was used to protect the exocyclic amines of the heterocyclic bases of A and C PNA monomers and the backbone primary amine was protected with the monomethoxytrityl group. The thymine and cytosine PNA monomers were used in conjunction with std. DNA synthesis monomers to produce chimeric PNA-DNA (PDC) oligomers. UV melting studies confirmed that these oligomers form stable hybrids with complementary DNA strands and that mismatches in the DNA but more so in the PNA sections lead to duplex destabilization.

IT **23124-10-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and properties of DNA-peptide nucleic acid (DNA-PNA) chimeric oligomers)
RN 23124-10-9 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, methyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 54 OF 116 CAPLUS COPYRIGHT 2002 ACS
1996:580596 Document No. 125:329293 Preparation of .beta.-lactam nucleic acids. Ravikumar, Vasulinga; Mohan, Venkatraman (Isis Pharmaceuticals, Inc., USA). U.S. US 5554746 A 19960910, 18 pp. (English). CODEN: USXXAM. APPLICATION: US 1994-243368 19940516.

GI



I

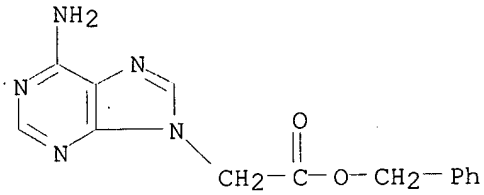
Searched by: Mary Hale 308-4258 CM-1 12D16

AB .beta.-Lactam monomers [I; A = [C(R6)R7]x; R6, R7 = H, alkyl, aryl, alkyl (un)substituted NH2, etc.; x = 0-10; B = adenine, guanine, thymine, cytosine, uracil; E1, E2 = H, OH-protecting group; m, n = 0-6], which can be joined into oligomeric compds. such as via preferred phosphate linkages including phosphodiester and phosphorothioate linkages, which are useful as diagnostic and research reagents (no data), are prepd.

IT **183181-27-3P 183181-59-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of .beta.-lactam nucleic acids)

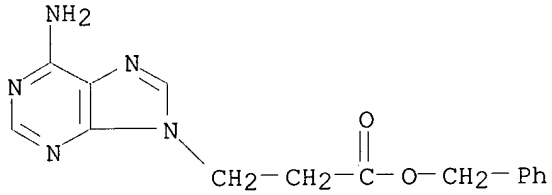
RN 183181-27-3 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 183181-59-1 CAPLUS

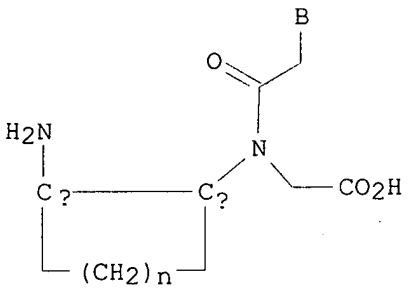
CN 9H-Purine-9-propanoic acid, 6-amino-, phenylmethyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 55 OF 116 CAPLUS COPYRIGHT 2002 ACS

1996:534869 Document No. 125:196392 Preparation of peptide nucleic acid incorporating a chiral backbone. Nielsen, Peter E.; Buchardt, Ole; Lagriffoul, Pierre (Buchardt, Dorte, Den.). PCT Int. Appl. WO 9620212 A2 19960704, 67 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1995-IB1169 19951228. PRIORITY: US 1994-366231 19941228.

GI



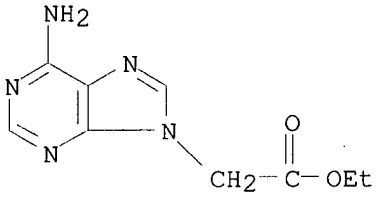
I

AB A novel class of peptide nucleic acid monomers I (B = nucleobase, n = 0-3, C.alpha. and/or C.beta. is S configuration) are synthesized having chirality in the backbone. Peptide nucleic acid and oligomers are synthesized to incorporate these chiral monomers.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of peptide nucleic acid incorporating a chiral backbone)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 56 OF 116 CAPLUS COPYRIGHT 2002 ACS

1996:455767 Document No. 125:115148 Synthesis of peptide nucleic acid conjugates. Nielsen, Peter; Egholm, Michael; Buchardt, Ole; Sonnechsen, Soren Holst; Lohse, Jesper; Manoharan, Muthiah; Kiely, John; Griffith, Michael; Sprankle, Kelly (Isis Pharmaceuticals, Inc., USA; Buchardt, Dorte). PCT Int. Appl. WO 9611205 A1 19960418, 196 pp. DESIGNATED STATES: W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1995-US12931 19951006. PRIORITY: US 1994-319411 19941006.

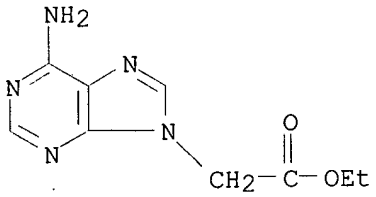
AB Synthesis of a novel class of peptide nucleic acids is reported. The peptide nucleic acids generally comprise ligands such as naturally occurring DNA bases attached to a peptide backbone through a suitable linker.

IT **25477-96-7P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation)
(synthesis of peptide nucleic acid conjugates)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16



L27 ANSWER 57 OF 116 CAPLUS COPYRIGHT 2002 ACS

1996:265320 Document No. 124:317794 Peptide nucleic acids and bis-peptide nucleic acids containing C-pyrimidines and isopyrimidines. Egholm, Michael; Nielsen, Peter; Buchardt, Ole; Dueholm, Kim L.; Christensen, Leif; Coull, James M.; Kiely, John; Griffith, Michael (Isis Pharmaceuticals, Inc., USA; Perseptive Biosystems; Buchardt, Dorte). PCT Int. Appl. WO 9602558 A1 19960201, 115 pp. DESIGNATED STATES: W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TT, UA; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1995-US9084 19950713. PRIORITY: US 1994-275951 19940715.

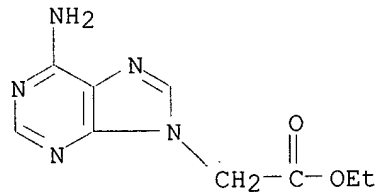
AB Novel peptide nucleic acids and novel linked peptide nucleic acids, form triple stranded structures with nucleic acids. The peptide nucleic acids include ligands such as naturally occurring nucleobases attached to a peptide backbone through a suitable linker. Other nucleobases including C-pyrimidines and iso-pyrimidines can be used as the ligands in Hoogsteen strands to increase binding affinity. Two peptide nucleic acid strands are joined together with a linker to form a bis-peptide nucleic acid. The individual strands of the peptide nucleic acids in the bis compds. can be oriented either parallel or antiparallel to each other.

IT **25477-96-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (peptide nucleic acids and bis-peptide nucleic acids contg. C-pyrimidines and isopyrimidines)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 58 OF 116 CAPLUS COPYRIGHT 2002 ACS

1996:151879 Document No. 124:290251 Liquid phase synthesis of a peptidic nucleic acid dimer. Farese, Audrey; Patino, Nadia; Condom, Roger; Dalleu, Sandrine; Guedj, Roger (Laboratoire Chimie Bioorganique, Univ. Nice Sophia-Antipolis, Nice, F-06108, Fr.). Tetrahedron Lett., 37(9), 1413-16 (English) 1996. CODEN: TELEAY. ISSN: 0040-4039.

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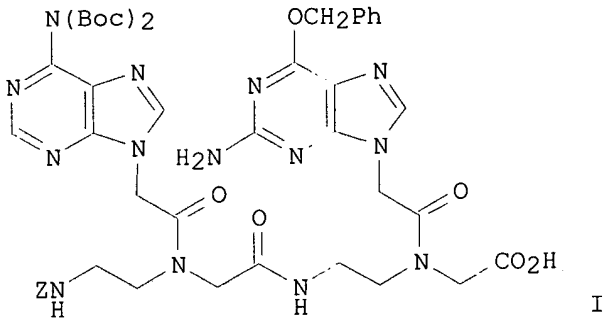
Searched by: Mary Hale 308-4258 CM-1 12D16



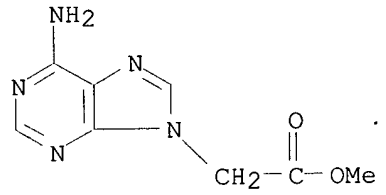
I

AB The first liq. phase synthesis of a peptide nucleic acid (PNA), dimer I (Boc = CO2CMe3, Z = PhCH2O2C) contg. guanine and adenine, has been achieved in good yields. A new strategy was elaborated in order to circumvent difficult coupling of the protected PNA.

IT **23124-10-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(liq. phase synthesis of a peptide nucleic acid dimer)

RN 23124-10-9 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, methyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 59 OF 116 CAPLUS COPYRIGHT 2002 ACS

1995:994345 Document No. 124:146851 Preparation of oligomeric peptide nucleic acid (PNA) combinatorial libraries and improved methods of synthesis. Cook, Philip Dan; Kiely, John; Sprankle, Kelly (Isis Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 9523163 A1 19950831, 103 pp. DESIGNATED STATES: W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1995-US2182 19950222. PRIORITY: US 1994-200742 19940223.

AB New sub-monomer synthetic methods for the prepn. of peptide nucleic acid oligomeric structures, useful as inhibitors of enzymes such as phospholipase A2 and for the treatment of inflammatory diseases including atopic dermatitis and inflammatory bowel disease (no data), are disclosed, that provide for the synthesis of both predefined sequence peptide nucleic acid oligomers as well as random sequence peptide nucleic acid oligomers. Further these methods also provide for the incorporation of peptide nucleic acid units or strings of such units with amino acids or strings of amino acids in chimeric peptide nucleic acid-amino acid compds. Further disclosed are methods of making random libraries of peptide nucleic acids using the fully preformed monomers. Thus, a combinatorial library of chimeric peptide nucleic acid oligomers was prepd. using 1-[(N2-benzyloxycarbonyl-N6-benzyloxy-2-aminopurin-9-yl)acetyl]-2-oxomorpholine (I), 1-[(N6-benzyloxycarbonyladenin-9-yl)acetyl]-2-

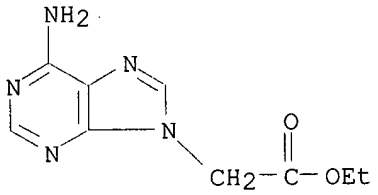
oxomorpholine (II), 1-[(N4-benzyloxycarbonylcytosin-1-yl)acetyl]-2-oxomorpholine (III), and 1-(thymin-1-ylacetyl)-2-oxomorpholine (IV), which involved coupling of IV to a MBHA resin, Mitsunobu reaction of the resulting N-(thymin-1-ylacetyl)-N-(2-hydroxyethyl)glycine-MBHA resin with (Boc)2NH using Ph3P and di-Et azodicarboxylate, random coupling of the resulting N-(thymin-1-ylacetyl)-N-(2-aminoethyl)glycine-MBHA resin with a mixt. of I, II, III, and IV followed by Mitsunobu reaction for converting the terminal hydroxy group to the terminal amine moieties, repeating the latter procedure for extension of backbone and addn. of further nucleoside bases to complete the oligomer of the desired length, addn. of a peptide to the peptide nucleic acid unit using std. solid phase Merrifield peptide synthesis, and cleavage of peptide nucleic acid oligomers from the resin.

IT **25477-96-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of oligomeric peptide nucleic acid (PNA) combinatorial libraries and improved methods of synthesis)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 60 OF 116 CAPLUS COPYRIGHT 2002 ACS

1995:986305 Document No. 124:30274 Preparation of pyrrolidine-containing monomers and oligomers.. Acevedo, Oscar L.; Hebert, Normand (Isis Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 9518792 A1 19950713, 96 pp. DESIGNATED STATES: W: CA, JP, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1995-US356 19950111. PRIORITY: US 1994-180134 19940111.

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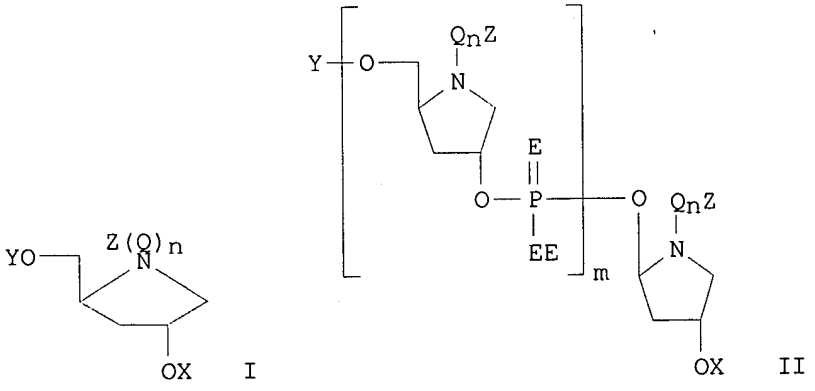


AB Monomers (I; X = H, phosphate, activated phosphate, activated phosphite, solid support; Y = H, protecting group; Z = L1, L1G1, L2G2, NR3R4, N-heterocyclyl, purinyl, pyrimidinyl, phosphate, polyether residue,

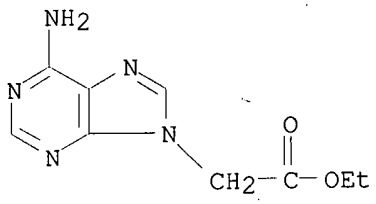
Searched by: Mary Hale 308-4258 CM-1 12D16

polyethylene glycol residue; L1 = alkyl, alkenyl, alkynyl; L2 = aryl, aralkyl; G1 = halo, OR1, SR2, NR3R4, CHO, CONR3R4, etc.; R1-R4 = H, alkyl, protecting group; Q = L1, G3, L1G3, G3L1G3; G3 = CO, CS, CO2, CONH, CSO, CSNH, SO2; n = 0, 1), and oligomers [II; X = H, phosphate, activated phosphate, activated phosphite, solid support, conjugate group, oligonucleotide residue; Y = H, protecting group, conjugate group, oligonucleotide residue; E = O, S; EE = O-, NYT; Y = H, (Q2)jZ2; T = (Q1)kZ1; YT = atoms to form a heterocycle; Q1, Q2 = alkyl, alkenyl, alkynyl, carbocyclyl, heterocyclyl, aralkyl, polyalkylglycol residue, etc.; j, k = 0, 1; Z1, Z2 = H, alkyl, alkenyl, alkynyl, aryl, aralkyl, halo, CHO, OR1, SR2, NR3R4, CONR3R4, reporter group, metal coordination group, N-heterocyclyl, etc; m = 1-50; n = 0,1; Q = alkyl, acyl, CO2, CSO, CSNH, SO2, etc.; Z = alkyl, alkenyl, alkynyl, aryl, OR1, SR2, CONR3R4, OH, SH, SMe, phosphate, metal coordination group, etc.], were prepd. Oligomer libraries were prepd. and found to inhibit phospholipase A2 and leukotriene B4 with IC50 = 1.5 .mu.M and 2.0 .mu.M, resp.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pyrrolidine-contg. monomers and oligomers)

RN 25477-96-7 CAPLUS

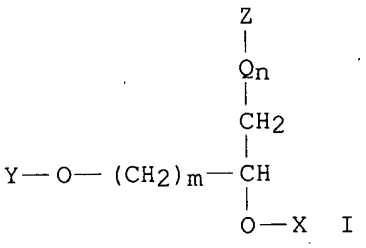
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 61 OF 116 CAPLUS COPYRIGHT 2002 ACS

1995:982328 Document No. 124:30276 Synthesis of acyclic oligonucleotides as antiviral and antiinflammatory agents and inhibitors of phospholipase A2. Cook, Phillip Dan; Acevedo, Oscar L.; Davis, Peter W.; Ecker, David J.; Hebert, Normand (Isis Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 9518820 A1 19950713, 126 pp. DESIGNATED STATES: W: CA, JP, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1995-US449 19950111. PRIORITY: US 1994-179970 19940111.

GI



AB Title ethylene glycol acyclic oligonucleotides I (Q = alkyl, alkenyl, alkynyl, alkylamino, ester amide, thio ester, imine, sulfonyl; X = H, PO3H2, polymer support; Y = H, protected hydroxyl; Z = nucleobase,

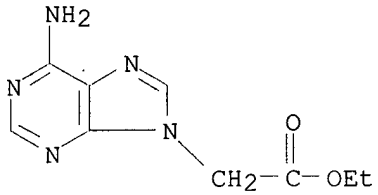
Searched by: Mary Hale 308-4258 CM-1 12D16

polyether, polyethylene glycol, N-contg. heterocycle; n = 0, Z = nucleobase, alkylamine; m = 1-6) were prepd. as antiviral and antiinflammatory agents and inhibitors of phospholipase A2.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of acyclic oligonucleotides as antiviral and antiinflammatory agents and inhibitors of phospholipase A2)

RN 25477-96-7 CAPLUS

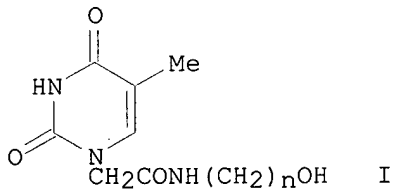
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 62 OF 116 CAPLUS COPYRIGHT 2002 ACS

1995:725612 Document No. 123:285619 Acyclic nucleoside analogs with an amide bond. Mikhailov, S. N.; Efimtseva, E. V.; Fomicheva, M. V.; Rodionov, M. S.; Kern, E. R. (Engelhardt Inst. Mol. Biol., Russian Acad. Sci., Moscow, Russia). Bioorg. Khim., 21(2), 130-2 (Russian) 1995. CODEN: BIKHD7. ISSN: 0132-3423.

GI



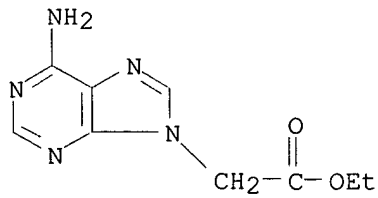
I

AB Thymine-contg. amides I (n = 2, 3, 4) were prepd. by reaction of thymine with BrCH2COOEt, followed by reaction of the esters with H2N(CH2)nOH. The cytosine and adenine analogs were similarly prepd. The amides have no anti-HIV, antiherpetic, or cytotoxic activity.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and amidation of)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 63 OF 116 CAPLUS COPYRIGHT 2002 ACS

Searched by: Mary Hale 308-4258 CM-1 12D16

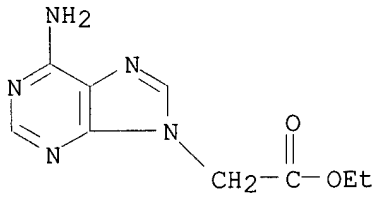
1995:630997 Document No. 123:257211 Acyclic nucleoside and nucleotide analogs with amide bond. Efimtseva, E. V.; Mikhailov, S. N.; Jasko, M. V.; Malakhov, D. V.; Semizarov, D. G.; Fomicheva, M. V.; Kern, E. R. (Engelhardt Institute Molecular Biology, Russian Academy Science, Moscow, 117984, Russia). Nucleosides Nucleotides, 14(3-5), 373-5 (English) 1995. CODEN: NUNUD5. ISSN: 0732-8311.

AB A series of acyclic nucleosides and related .alpha.-phosphonyl acyclic analogs of dNTP with an amide bond have been prepd. Their antiviral and and cytotoxicity were investigated (no data).

IT **25477-96-7**
RL: RCT (Reactant)
(prepn. and antiviral activity of acyclic nucleoside and nucleotide analogs with amide bond)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 64 OF 116 CAPLUS COPYRIGHT 2002 ACS

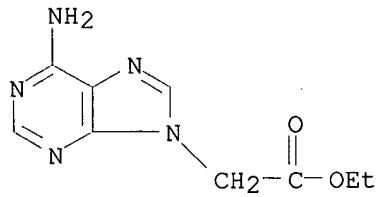
1994:668369 Document No. 121:268369 Ethyl 9-adeninylacetate at 122 K. Flensburg, Claus; Egholm, Michael (Cent. Crystallographic Studies, Univ. Copenhagen, Copenhagen, DK-2100, Den.). Acta Crystallogr., Sect. C: Cryst. Struct. Commun., C50(9), 1480-2 (English) 1994. CODEN: ACSCEE. ISSN: 0108-2701.

AB The title compd. is orthorhombic, space group Pbca, with a 19.4943(15), b 12.2427(7), and c 8.5428(5) .ANG.; Z = 8, dc = 1.441; R(F) = 0.0318, Rw(F2) = 0.0856 for 2105 reflections. At. coordinates are given. The Et acetate moiety is virtually planar and almost perpendicular to the adenine ring system. H bonds between the amino groups and 2 adenine N atoms connect the mols. in chains parallel to the c axis.

IT **25477-96-7**, Ethyl 9-adeninylacetate
RL: PRP (Properties)
(crystal structure of)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 65 OF 116 CAPLUS COPYRIGHT 2002 ACS

1994:606011 Document No. 121:206011 Synthesis of Peptide Nucleic Acid Monomers Containing the Four Natural Nucleobases: Thymine, Cytosine, Adenine, and Guanine and Their Oligomerization. Dueholm, Kim L.; Egholm, Michael; Behrens, Carsten; Christensen, Leif; Hansen, Henrik F.; Vulpius, Tore; Petersen, Kenneth H.; Berg, Rolf H.; Nielsen, Peter E.; Buchardt,

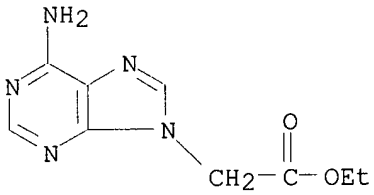
Ole (H. C. Oersted Institute, University of Copenhagen, Copenhagen, DK-2100, Den.). J. Org. Chem., 59(19), 5767-73 (English) 1994. CODEN: JOCEAH. ISSN: 0022-3263.

AB The prepn. of mixed-sequence peptide nucleic acids (PNAs) contg. the four natural nucleobases (thymine, cytosine, adenine, and guanine) is described. The PNA monomers contg. thymine, benzyloxycarbonyl (Cbz)-protected cytosine or adenine, or benzyl-protected guanine were prepd. via convergent syntheses. Subsequent to introduction of a carboxymethyl linker at N-1 of the pyrimidines or N-9 of the purines and suitable protection of exocyclic groups, the nucleobase derivs. were coupled to the tert-butoxycarbonyl (Boc)-protected backbone esters BocNHCH2CH2NHCH2CO2R (R = Me, Et) and finally hydrolyzed affording the monomers BocNHCH2CH2N(COCH2B)CH2CO2H (B = nucleobase). Two mixed-sequence 10-mers, each with five purines incorporated, and a mixed-sequence 15-mer contg. seven purines were assembled essentially following std. solid phase peptide synthesis protocols.

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of peptide nucleic acid monomers contg. the four natural nucleobases and their oligomerization)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 66 OF 116 CAPLUS COPYRIGHT 2002 ACS

1994:135140 Document No. 120:135140 Peptide nucleic acids and their effect on genetic material. Thomson, Stephen A.; Noble, Stewart A.; Ricca, Daniel J. (Glaxo Inc., USA). PCT Int. Appl. WO 9312129 A1 19930624, 49 pp. DESIGNATED STATES: W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, UA, US; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1992-US10921 19921217. PRIORITY: US 1991-809661 19911218.

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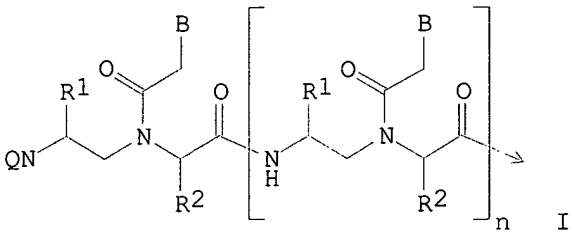
Searched by: Mary Hale 308-4258 CM-1 12D16



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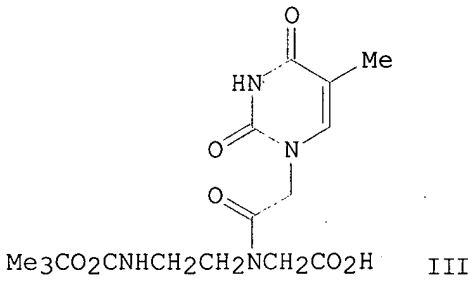


III

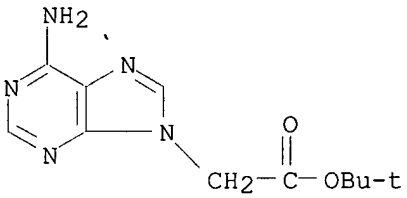
AB Nucleic acid base-contg. peptides I [B = nucleic acid base; Q, J = protective group; QJ = bond; R1, R2 = H, (un)substituted alkyl, aryl, heteroaryl; n= .gtoreq.1] were prepd. for use as inhibitors of genetic transcription. Thus, I [Q, R1, R2 = H, J = NH2, B = thymine; n = 5, II] was prepd. from resin-bound lysine and the monomer III which was obtained by reductive alkylation of H2NCH2CO2Me.HCl with Me3CO2CNHCH2CHO, followed by reaction with 1-carboxymethylthymine. II inhibited poly rA.T25-30 duplex formation at .gtoreq.0.1 .mu.M.

IT **152774-16-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(intermediate in prepn. of nucleic acid base-contg. peptides)

RN 152774-16-8 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 67 OF 116 CAPLUS COPYRIGHT 2002 ACS

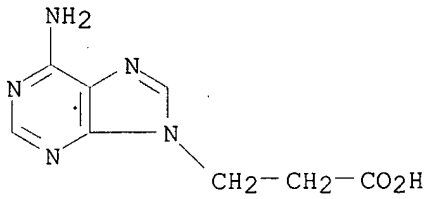
1993:650359 Document No. 119:250359 Synthesis of adenine derivatives by solid-liquid phase-transfer catalysis. Wang, Zhicai; Lin, Dianwei; Zheng, Qihuang (Dep. Chem., Zhongshan Univ., Guangzhou, 510275, Peop. Rep. China). Yingyong Huaxue, 10(3), 42-6 (Chinese) 1993. CODEN: YIHUED. OTHER SOURCES: CASREACT 119:250359.

AB Adenine derivs. eritadenine, Et 4-(6-amino-9H-purin-9-yl)-2(R),3(R)-dihydroxybutyrate, .beta.-adenylpropionic acid and Et .beta.-adenylpropionate have been synthesized from adenine by solid-liq. phase transfer catalysis. The effects of reaction conditions on the yields were studied. The results showed that PEG is a good phase transfer catalyst for the reaction.

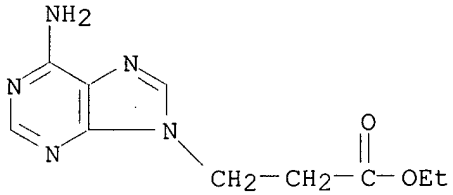
IT **4244-47-7P 7083-40-1P**

Searched by: Mary Hale 308-4258 CM-1 12D16

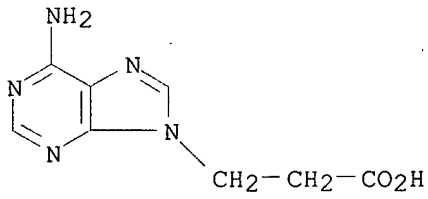
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



RN 7083-40-1 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



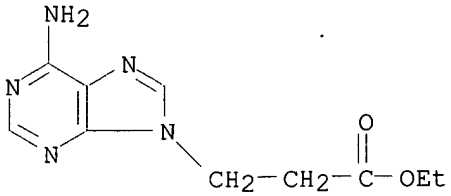
L27 ANSWER 68 OF 116 CAPLUS COPYRIGHT 2002 ACS
1993:626330 Document No. 119:226330 Preparation of PVA membrane containing nucleic acid analogs and studies on separation of nucleosides and dinucleotides using this membrane. Wada, Takehiko; Chirachianchai, Suwabun; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Mol. Cryst. Liq. Cryst. Sci. Technol., Sect. A, 219, 169-72 (English) 1992. CODEN: MCLCE9. ISSN: 1058-725X.
AB PVA membranes contg. nucleic acid analogs were prepd. Sepn. of nucleosides and dinucleotides were studied using these membranes. In the case of PVA membranes contg. thymine base, selective diffusion of adenosine, which is the complementary Watson-Crick base pair of thymine, was obsd. This may be caused by specific base-base interaction between thymine and adenine.
IT **4244-47-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



IT **7083-40-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)
RN 7083-40-1 CAPLUS

Searched by: Mary Hale 308-4258 CM-1 12D16

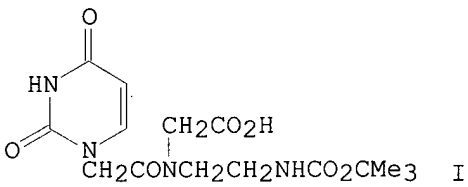
CN 9H-Purine-9-propanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 69 OF 116 CAPLUS COPYRIGHT 2002 ACS

1993:581235 Document No. 119:181235 Peptide nucleic acids. Buchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik (Den.). PCT Int. Appl. WO 9220702 A1 19921126, 192 pp. DESIGNATED STATES: W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1992-EP1219 19920522. PRIORITY: DK 1991-986 19910524; DK 1991-987 19910524; DK 1992-510 19920415.

GI

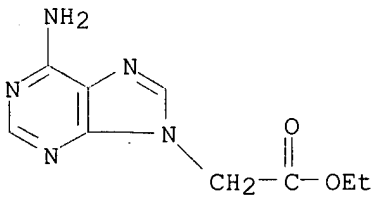


AB Peptides contg. nucleic acid bases were prepd. These peptides formed stable hybrids with oligonucleotides. Thus, H2NCH2CH2NHCH2CO2H was tert-butoxycarbonylated and treated with N1-carboxymethylthymine pentafluorophenyl ester to give the thymine deriv. Boc-Taeg-OH (I). I was used in the solid-phase synthesis of H-[Taeg]10-Lys-NH2 which formed a hybrid with (dA)10 which had a melting temp. of 73.degree..

IT **25477-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and benzyloxycarbonylation of)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 70 OF 116 CAPLUS COPYRIGHT 2002 ACS

Searched by: Mary Hale 308-4258 CM-1 12D16

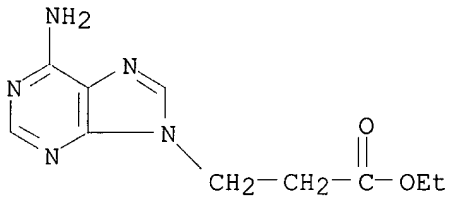
1993:559963 Document No. 119:159963 Characterisation of adducts of nucleic bases and acrylic monomers. Crippa, Sergio; Di Gennaro, Patrizia; Lucini, Ruggero; Orlandi, Marco; Rindone, Bruno (Dip. Chim. Org. Ind., Univ. Milano, Milan, I-20133, Italy). Gazz. Chim. Ital., 123(4), 197-203 (English) 1993. CODEN: GCITA9. ISSN: 0016-5603.

AB Spectral data and thermodn. calcns. of adducts of guanine, adenine, thymine, and uracil with acrylonitrile, Et acrylate and Et crotonate are reported. Purine adducts derive from attack at N-7 and N-9, and pyrimidine adducts derive from attack at N-1. Acrylonitrile also forms N-1,N-3 bis adducts with pyrimidines. Structural assignment was by 1H and 13C NMR and using COSY-RELAY and NOE effects. Force-field calcns. indicated the most stable conformations of the reaction products.

IT **7083-40-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 7083-40-1 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 71 OF 116 CAPLUS COPYRIGHT 2002 ACS

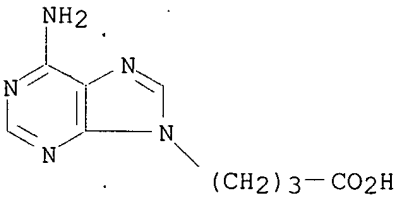
1993:517014 Document No. 119:117014 Porphyrins coupled with nucleoside bases. Synthesis and some properties of guanine, cytosine and adenine-thymine derivatives. Hisatome, Masao; Maruyama, Noriaki; Ikeda, Koichi; Yamakawa, Koji (Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan). Heterocycles, 36(3), 441-4 (English) 1993. CODEN: HTCYAM. ISSN: 0385-5414.

AB Synthesis of several porphyrin derivs. having a guanine, cytosine or adenine-thymine pair is described. Diamagnetic shift behaviors of the base proton signals in the 1H NMR spectra of the derivs. and hypochromism of the Soret band in the electronic spectra are briefly discussed.

IT **33147-28-3**
RL: RCT (Reactant)
(condensation of, with porphyrins)

RN 33147-28-3 CAPLUS

CN 9H-Purine-9-butanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 72 OF 116 CAPLUS COPYRIGHT 2002 ACS

1992:15822 Document No. 116:15822 Multifunctional pharmaceutical compounds and methods of use. Glasky, Alvin J. (USA). PCT Int. Appl. WO 9114434 A1 19911003, 65 pp. DESIGNATED STATES: W: AU, BR, CA, FI, HU, JP, KR, MC,

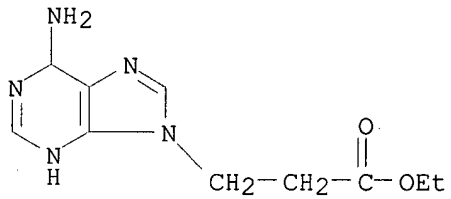
NO, SU; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1991-US2066 19910326. PRIORITY: US 1990-500789 19900328.

AB Multifunctional pharmaceuticals comprise .gtoreq.2 biol. active chem. groups linked by a chem. bridging group. The compds. are useful for treating degenerative diseases and interrelated physiol. systems. 3-(1,6-Dihydro-6-oxo-9H-purin-9-yl)propanoic acid (AIT-0080) enhanced T-lymphocyte proliferation at a moderate dosage (10 .mu.g/mL), yet enhanced B-lymphocyte function at relatively low dosage (1 .mu.g/mL). Addnl., AIT-0080 enhanced memory function as well as locomotor activity at 0.5 mg/kg in vivo. AIT-0080 was prepd. from adenine in 3 steps.

IT **138137-08-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in multifunctional pharmaceutical prepn.)

RN 138137-08-3 CAPLUS

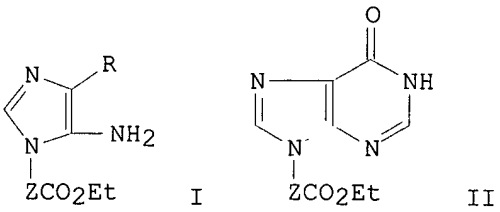
CN 9H-Purine-9-propanoic acid, 6-amino-1,6-dihydro-, ethyl ester (9CI) (CA INDEX NAME)

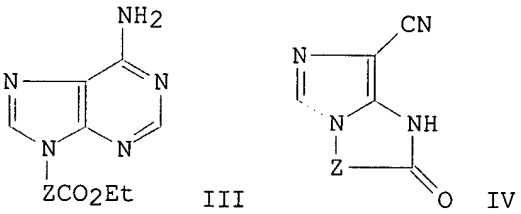


L27 ANSWER 73 OF 116 CAPLUS COPYRIGHT 2002 ACS

1991:207183 Document No. 114:207183 Synthesis and intramolecular cyclization of 5-aminoimidazolealkanoates and their conversion to purine derivatives. Birkett, Paul R.; Chapleo, Christopher B.; Mackenzie, Grahame (Humberside Coll. Higher Educ., Hull, HU6 7RT, UK). Synthesis (2), 157-9 (English) 1991. CODEN: SYNTBF. ISSN: 0039-7881. OTHER SOURCES: CASREACT 114:207183.

GI





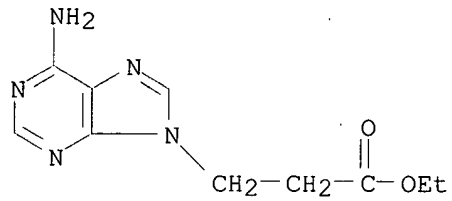
AB Reaction of EtOCH:NCHRCN (R = CONH2, cyano) with EtO2CZNH2.HCl [Z = CH2, CH2CH2, CHMe) in presence of Et3N gave 55-69% aminoimidazolylalkanoates I.

Searched by: Mary Hale 308-4258 CM-1 12D16

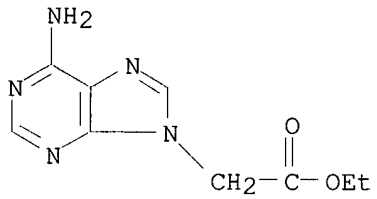
Cyclization of I (R = CONH2) with HC(OEt)3 in DMF gave hypoxanthines II. Adenines III were obtained by the reaction of I (R = cyano) with HC(OEt)3 in EtOH, followed by 1 mol. equiv. NH3. Reaction of I (R = cyano) with ethanolic Et3N to give imidazoimidazoles or imidazopyrimidine IV (Z = CH2, CHMe, CH2CH2).

IT **7083-40-1P 25477-96-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 7083-40-1 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



RN 25477-96-7 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 74 OF 116 CAPLUS COPYRIGHT 2002 ACS
1991:101481 Document No. 114:101481 Porphyrins coupled with nucleoside bases. Synthesis and characterization of adenine- and thymine-porphyrin derivatives. Hisatome, Masao; Maruyama, Noriaki; Furutera, Tetsuo; Ishikawa, Tomoyasu; Yamakawa, Koji (Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan). Chem. Lett. (12), 2251-4 (English) 1990. CODEN: CMLTAG. ISSN: 0366-7022.

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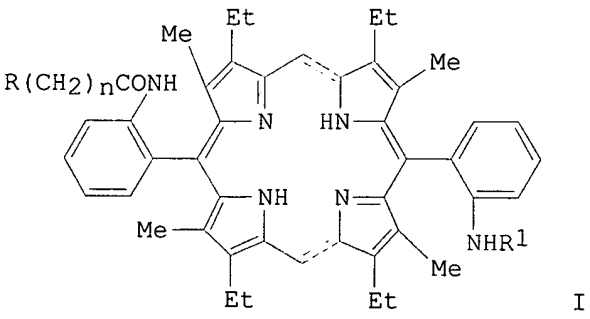

I

AB Porphyrins I (R = adenyl, thyminyl; R1 = H, CO2Et, CO2CH2Ph; n = 3, 4)

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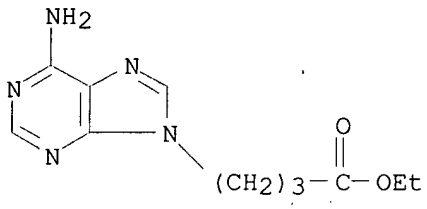
have been synthesized. Spectroscopic study suggested an interaction between the porphyrin ring and the base moiety, and indicated nucleoside base recognition ability of the compds.

IT **41785-06-2**
RL: RCT (Reactant)
(base pairing of, with thyminylalkanoylaminophenylporphyrin)

RN 41785-06-2 CAPLUS

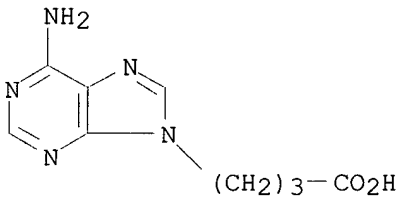
CN 9H-Purine-9-butanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



IT **33147-28-3 90973-36-7**
RL: RCT (Reactant)
(reaction of, with aminophenylporphyrin)

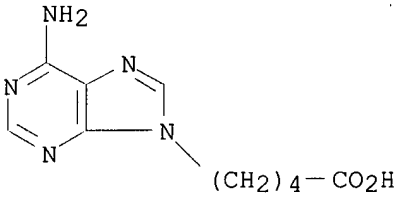
RN 33147-28-3 CAPLUS

CN 9H-Purine-9-butanoic acid, 6-amino- (9CI) (CA INDEX NAME)



RN 90973-36-7 CAPLUS

CN 9H-Purine-9-pentanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 75 OF 116 CAPLUS COPYRIGHT 2002 ACS

1991:43429 Document No. 114:43429 Synthesis and interaction of water-soluble nucleic acid analogs. Takemoto, Kiichi; Wada, Takehiko; Mochizuki, Eiko; Inaki, Yoshiaki (Fac. Eng., Osaka Univ., Osaka, Japan). Polym. Mater. Sci. Eng., 62, 558-62 (English) 1990. CODEN: PMSEDG. ISSN: 0743-0515.

AB Water sol. polyethyleneimine derivs. contg. both nucleic acid bases and homoserine were prepd. The polyethyleneimine derivs. formed 1:1 complex by complementary base pairing in aq. soln. These polymers also formed polymer complexes with polynucleotides by specific interaction between complementary nucleic acid bases.

IT **4244-47-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with aminobutanamide)

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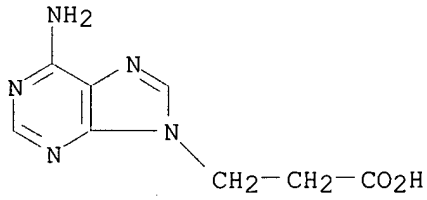
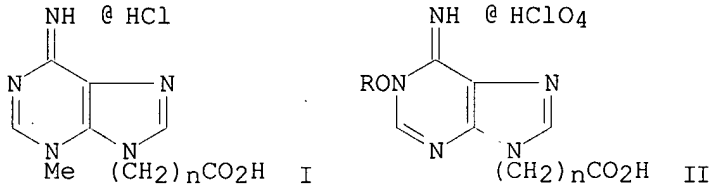
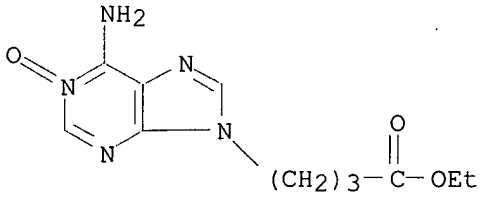
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 76 OF 116 CAPLUS COPYRIGHT 2002 ACS
1990:591038 Document No. 113:191038 Purines. XL. Preparation of 9-(.omega.-carboxyalkyl)-3-methyladenines. Fujii, Tozo; Saito, Tohru; Kumazawa, Yukinari (Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan). Chem. Pharm. Bull., 38(5), 1392-5 (English) 1990. CODEN: CPBTAL. ISSN: 0009-2363. OTHER SOURCES: CASREACT 113:191038.
GI

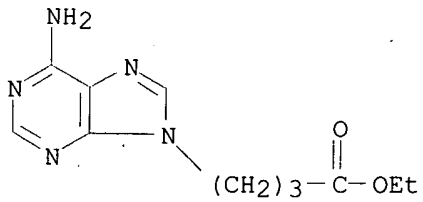


AB With a view to supplying haptens to be connected to carrier proteins for raising antibodies to 3-methyl-2'-deoxyadenosine and/or 3-methyladenine, the title compds. I (n = 1, 3) have been prepd. from 1-alkoxy-9-(.omega.-carboxyalkyl)adenine salts II (n = 1, R = Et; n = 3, R = Me).
IT **130080-69-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and methylation of)
RN 130080-69-2 CAPLUS
CN 9H-Purine-9-butanoic acid, 6-amino-, ethyl ester, 1-oxide (9CI) (CA INDEX NAME)



IT **41785-06-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and oxidn. of)
RN 41785-06-2 CAPLUS
CN 9H-Purine-9-butanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16



L27 ANSWER 77 OF 116 CAPLUS COPYRIGHT 2002 ACS
1990:459751 Document No. 113:59751 Orientation, recognition, and photoreaction of nucleolipids in model membranes. Ahlers, M.; Ringsdorf, H.; Rosemeyer, H.; Seela, F. (Inst. Org. Chem., Univ. Mainz, Mainz, 6500, Fed. Rep. Ger.). Colloid Polym. Sci., 268(2), 132-42 (English) 1990. CODEN: CPMSB6. ISSN: 0303-402X.

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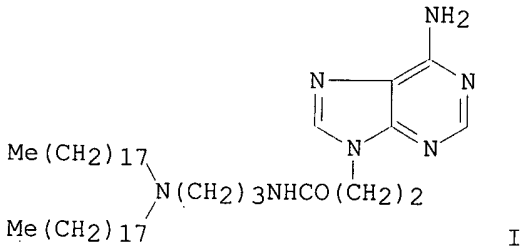


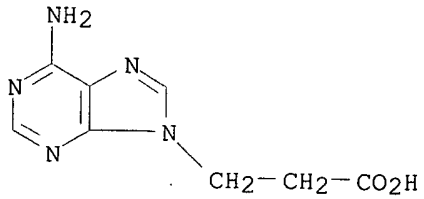
I

AB Amphiphiles with nucleobases and nucleosides as headgroups, e.g., I, have been synthesized. Their surface behavior was investigated in monolayers at the air/water interface. The double chain nucleolipids form stable monolayers with nearly identical surface pressure-area diagrams, whereas the spreading behavior of the mono chain amphiphiles is dominated by the various nucleobase-headgroups. When measuring the interactions between nucleolipid monolayers and nucleobases (monomeric and polymeric ones), specific base-base effects could be obsd.: the complementary nucleobases solubilized in the subphase expand the monolayer more than the non-complementary ones. Photodimerization reactions of thymine-amphiphiles were investigated in mono- and multilayers as well as in spin-coated films.

IT **4244-47-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acylation of, with nitrophenol)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 78 OF 116 CAPLUS COPYRIGHT 2002 ACS

Searched by: Mary Hale 308-4258 CM-1 12D16

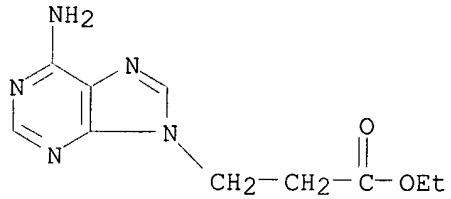
1989:633438 Document No. 111:233438 Nucleic acid analogs for high-performance liquid chromatography. Inaki, Yoshiaki; Nagae, Suguru; Miyamoto, Takashi; Sugiura, Yoshihiko; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Polym. Sci. Technol. (Plenum), 38(Appl. Bioact. Polym. Mater.), 185-204 (English) 1988. CODEN: POSTB5. ISSN: 0093-6286.

AB Nucleic acid base and nucleoside derivs. were bonded to 3-aminopropyl-silanized silica (APS-silica) and silica gel. These resins were useful as the columns of high performance liq. chromatog. (HPLC) for the selective sepn. of oligoethylenimine derivs. having pendant thymine or adenine bases. These column systems were also applicable to the sepn. of nucleosides, nucleotides, and oligonucleotides.

IT **7083-40-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to hypoxanthine deriv.)

RN 7083-40-1 CAPLUS

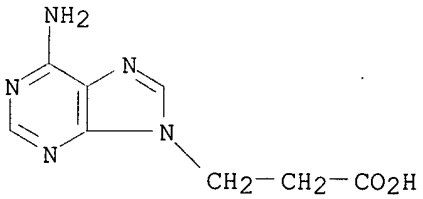
CN 9H-Purine-9-propanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



IT **4244-47-7DP**, silica gel bonded or reactions with poly-L-lysine derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, HPLC resin for sepn. of nucleic acid base derivs., nucleosides, nucleotides, and oligonucleotides)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 79 OF 116 CAPLUS COPYRIGHT 2002 ACS

1989:193309 Document No. 110:193309 Functional monomers and polymers. CLXXIII. Immobilization of nucleic acid bases on silica gel and application to HPLC for selective separation of nucleosides. Nagae, Suguru; Miyamoto, Takashi; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Polym. J. (Tokyo), 21(1), 19-33 (English) 1989. CODEN: POLJB8. ISSN: 0032-3896.

AB Nucleic acid base derivs. were immobilized on 3-aminopropylsilanized silica (APS-silica) and silica gel. The bases immobilized were thymine, uracil, cytosine, adenine, guanine, and hypoxanthine. These silica gels were proved to be useful as columns of high performance liq. chromatog. (HPLC) for the selective sepn. of nucleosides using specific interaction between complementary bases.

IT **4244-47-7DP**, polymer-bound
RL: SPN (Synthetic preparation); PREP (Preparation)

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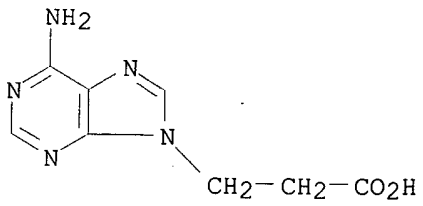
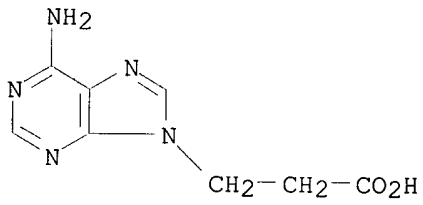
(prepn. of, for HPLC of nucleosides)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 80 OF 116 CAPLUS COPYRIGHT 2002 ACS
1989:8563 Document No. 110:8563 Nucleic acid analogs: their specific interaction and applicability. Takemoto, K.; Inaki, Y. (Fac. Eng., Osaka Univ., Osaka, 565, Japan). Polym. Mater. Sci. Eng., 58, 250-3 (English) 1988. CODEN: PMSEDG. ISSN: 0743-0515.
AB The prepn. and properties of polymers contg. nucleosides or nucleic acid bases attached to poly-L-lysine, poly-L-glutamic acid or polyethyleneimine are reported.
IT **4244-47-7D**, polylysineamide deriv.
RL: RCT (Reactant)
(reaction of, with (benzyloxycarbonyl)lysine and polylysine)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



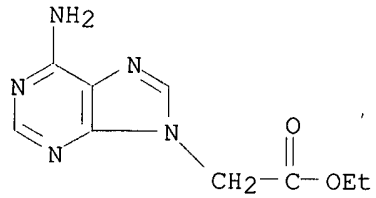
L27 ANSWER 81 OF 116 CAPLUS COPYRIGHT 2002 ACS
1988:544554 Document No. 109:144554 Sterilization of Pyrrhocoris apterus by open-chain nucleoside analogs: dose-response and structure-activity relationships. Slama, Karel; Holy, Antonin (Inst. Org. Chem. Biochem., Slovak Acad. Sci., Prague, 15800/5, Czech.). Acta Entomol. Bohemoslov., 85(2), 94-106 (English) 1988. CODEN: AEBOA9. ISSN: 0001-5601.
AB 93 Open-chain alkyl derivs. of nucleosides were tested for inhibition of female fecundity and hatching ability of the eggs. The oral assays included among others: N9-(2,3-dihydroxypropyl) derivs. of the heterocyclic bases; 9-alkyladenines with various (C2-C3) side chains; N9-polyhydroxyalkyladenines and N1-polyhydroxyalkyluracils (C4-C6); 3-(adenin-9-yl)-2-hydroxypropanoic acids and their derivs.; eritadenines and the addnl. 9-(carboxypolyhydroxyalkyl)adenines. The most active compd. was D-eritadenine. In drinking assays 7.5 .mu.g.cntdot.mL-1 of this compd. inhibited 50% larval hatching from the eggs; the IC50 value for the inhibition of female fecundity was 32 .mu.g.cntdot.mL-1. The action of some of the nucleotide analogs on insects closely paralleled ability of these compds. to suppress enzymic activity of SAH-hydrolase from rat liver. Exceptions to this rule were mostly related to generally toxic compds. or, esp., to 2'(3)'-O-phosphonylmethyl-9-(S)-(2,3-dihydroxypropyl) adenine, whose biol. activity depends on principles other than SAH-hydrolase inhibition. Thus, in addn. to their pronounced

antiviral effects, several compds. related to D-eritadenine or 3-adenin-9-yl-2-hydroxypropanoic acid appear to be selective insect sterilants or ovicides.

IT **25477-96-7**
RL: BIOL (Biological study)
(insect-sterilizing and ovicidal activity of, in Pyrrhocoris apterus, structure in relation to)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 82 OF 116 CAPLUS COPYRIGHT 2002 ACS

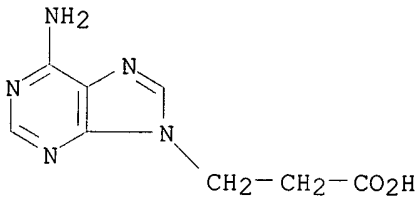
1987:156881 Document No. 106:156881 Functional monomers and polymers. CXXXI. Synthesis and interaction studies on polyacrylamide and polymethacrylamide derivatives containing nucleic acid bases. Inaki, Yoshiaki; Sugita, Shinichi; Takahara, Tohru; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). J. Polym. Sci., Part A: Polym. Chem., 24(12), 3201-17 (English) 1986. CODEN: JPACEC.

AB (Meth)acrylamide derivs. of nucleic acid bases were prepd. from the corresponding aminoethyl derivs. Free-radical polymn. of these monomers in water or in org. solvents gave their polymers. UV spectroscopy indicated that extremely stable polymer complexes were formed between complementary polymers contg. nucleic acid bases.

IT **4244-47-7**, 9-(2-Carboxyethyl)adenine
RL: RCT (Reactant)
(reaction of, with sodium azide in sulfuric acid)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 83 OF 116 CAPLUS COPYRIGHT 2002 ACS

1986:424556 Document No. 105:24556 Purines. XXVI. The Dimroth rearrangement of 9-substituted 1-methyladenines: accelerating effect of a .beta.-D-ribofuranosyl group at the 9-position. Fujii, Tozo; Saito, Tohru (Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan). Chem. Pharm. Bull., 33(9), 3635-44 (English) 1985. CODEN: CPBTAL. ISSN: 0009-2363. OTHER SOURCES: CASREACT 105:24556.

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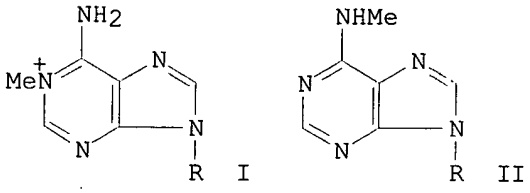
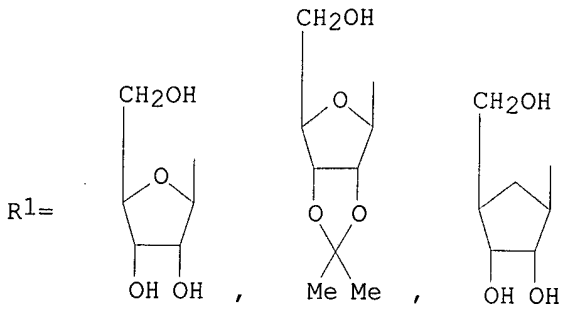
Searched by: Mary Hale 308-4258 CM-1 12D16

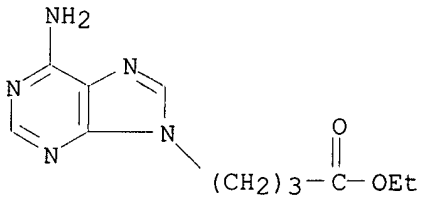




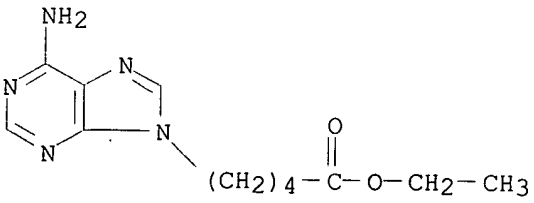
AB The reaction rates in the Dimroth rearrangements of 1-methyladenines I [R = Me, Et, CH2Ph2 (CH2)4OH, (CH2)5OH, R1] to purines II were measured in H2O at various pH's and ionic strength 1.0 and 40 .degree.C. In all cases, attack of hydroxide ion on the protonated species of I at the 2-position was faster than that on the neutral species by a factor of 90-180. I (R = .beta.-D-ribofuranosyl) was found to accelerate both modes of hydroxide attack most significantly. This rate enhancement is attributable solely to the electron-withdrawing effect of the furanose ring oxygen and not to the 5'-hydroxy group, a potential participant in intramol. catalysis for the hydroxide attack on the adenine ring at the 2-position.

IT **41785-06-2P 102788-98-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydride redn. of)

RN 41785-06-2 CAPLUS
CN 9H-Purine-9-butanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



RN 102788-98-7 CAPLUS
CN 9H-Purine-9-pentanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)



Searched by: Mary Hale 308-4258 CM-1 12D16

L27 ANSWER 84 OF 116 CAPLUS COPYRIGHT 2002 ACS

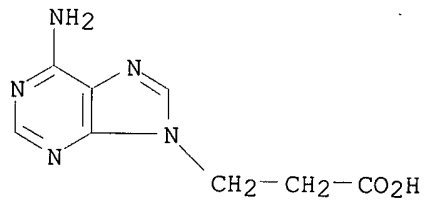
1986:402324 Document No. 105:2324 Polymer effects on the synthetic nucleic acid analogs. Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Makromol. Chem., Suppl., 14, 91-103 (English) 1985. CODEN: MCSUEU.

AB Polymer effects on the interaction of nucleic acid bases in oligomer models of synthetic nucleic acid analogs were studied. Oligomers of polyethyleneimine derivs. contg. nucleic acid bases were prepd. and UV spectra and photochem. reactions were studied in order to evaluate the intramol. and intermol. interactions between pendant nucleic acid bases in these compds. The intramol. interaction was caused by the nearest neighboring units and was independent of the remote units. The intramol. interaction was closely related to the intermol. interaction of the nucleic acid analogs and to the photodimerization of thymine bases in the oligomers and in the polymers.

IT **4244-47-7D**, reaction products with polyethyleneimine
RL: BIOL (Biological study)
(photodimerization of, monomers and polymers comparison with)

RN 4244-47-7 CAPLUS

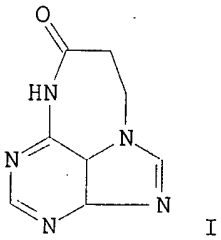
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 85 OF 116 CAPLUS COPYRIGHT 2002 ACS

1985:220644 Document No. 102:220644 Some intramolecular Michael additions of adenine derivatives. Brahme, Nanda M.; Smith, Walter T., Jr. (Dep. Chem., Univ. Kentucky, Lexington, KY, 45006-0055, USA). J. Heterocycl. Chem., 22(1), 109-12 (English) 1985. CODEN: JHTCAD. ISSN: 0022-152X. OTHER SOURCES: CASREACT 102:220644.

GI



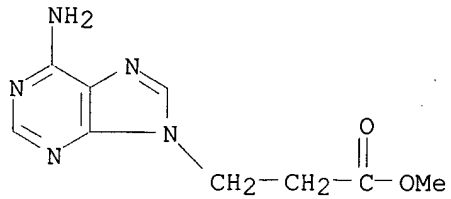
I

AB Reaction of adenine with acrylic anhydride or vinyl acrylate in Me2SO was accompanied by intramol. Michael addn. to give the diazepinopurine I which was hydrolyzed with 1N NaOH to give 7-carboxyethyladenine. Reaction of adenine with various acrylic derivs. in DMF or aq. NaOH gave 3-carboxyethyladenine. Adenine reacted with CH2:CHCN or Me acrylate in Me2SO to give a mixt. of the 7- and 9-substituted derivs.

IT **70259-15-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)

Searched by: Mary Hale 308-4258 CM-1 12D16

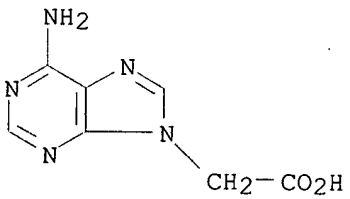
(prepn. of)
RN 70259-15-3 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 86 OF 116 CAPLUS COPYRIGHT 2002 ACS
1985:160066 Document No. 102:160066 Studies on S-adenosyl-L-homocysteine hydrolase. XIV. Structure-activity studies on open-chain analogs of nucleosides: inhibition of S-adenosyl-L-homocysteine hydrolase and antiviral activity. 2. Acid open-chain analogs. Holy, Antonin; Votruba, Ivan; De Clercq, Erik (Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10/6, Czech.). Collect. Czech. Chem. Commun., 50(1), 262-79 (English) 1985. CODEN: CCCCAK. ISSN: 0366-547X.

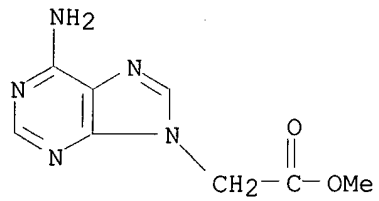
AB Over 50 .omega.-carboxyalkyl derivs. of adenine and other purine bases were examd. for their inhibitory effects on rat liver S-adenosyl-L-homocysteine hydrolase (I) [9025-54-1] and their antiviral activity. To be a I inhibitor the analog must contain an adenine base substituted at position 9 by an .omega.-carboxyalkyl (C3-C5) chain bearing .gtoreq. 1 OH function. The abs. configuration at the side-chain is decisive for the dihydroxy and trihydroxy compds., but less important for the monohydroxyalkanoic acids. D-Eritadenine (II) [23918-98-1] and 3-(adenin-9-yl)-2-hydroxypropanoic acid (III) [94535-32-7] are the most potent I inhibitors and the only compds. possessing antiviral activity (against vesicular stomatitis, parainfluenza type 3, reovirus type 1, and vaccinia virus). All these compds. effect a rapid irreversible inactivation of I. The esters of II and III exhibit little, if any inhibitory activity toward I; they are, however, much more potent antiviral agents than II and III, probably acting as prodrugs of the latter. 2-Amino-D-eritadenine [95973-21-0], (2R,3R)-5-(adenin-9-yl)-2,3-dihydroxypentanoic acid [95993-09-2], (9-(dicarboxymethyl)adenine [34573-03-0], 4-(adenin-9-yl)-2-hydroxybutanoic acid [53022-49-4], 3-(8-bromoadenin-9-yl)-2-hydroxypropanoic acid [95993-07-0], and O-carboxymethyl derivs. of 9-(2,3-dihydroxypropyl)- and 9-(2,3,4-trihydroxybutyl)adenine are described as novel compds.

IT **20128-29-4 23124-10-9**
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(virucidal activity of, adenosylhomocysteine hydrolase inhibition in relation to)
RN 20128-29-4 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)

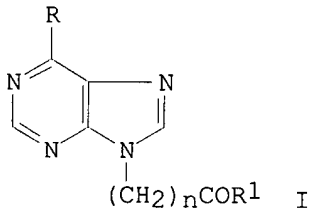


Searched by: Mary Hale 308-4258 CM-1 12D16

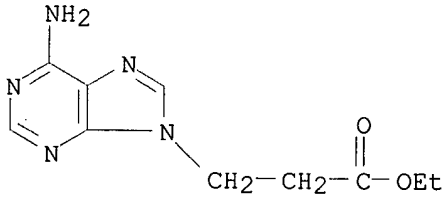
RN 23124-10-9 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, methyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 87 OF 116 CAPLUS COPYRIGHT 2002 ACS
1985:149749 Document No. 102:149749 Synthesis of modified amino acids containing purine bases of nucleic acids. Poritere, S.; Paegle, R.; Lidaks, M. (Inst. Org. Sint., Riga, 226006, USSR). Khim. Geterotsikl. Soedin. (1), 126-30 (Russian) 1985. CODEN: KGSSAQ. ISSN: 0453-8234. OTHER SOURCES: CASREACT 102:149749.
GI

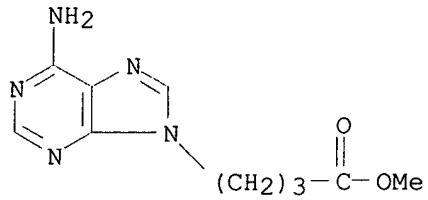


AB Adenylalkanoyl amino acids I [R = NH2, n = 1, 2, 3; R1 = NH(CH2)mCH(NH2)CO2H (m = 1-4), NH(CH2)mCO2H (m = 2, 3, 5), leucine, or phenylalanine residues] were prepd. from acids I (R1 = OH) via azides I (R1 = N3). Hypoxanthine analogs (I; R = OH, n = 1, 2; R1 = amino acid residue) were prepd. similarly.
IT **7083-40-1 23124-18-7 25477-96-7**
RL: RCT (Reactant)
(hydrazinolysis of)
RN 7083-40-1 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)

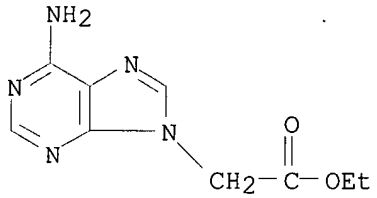


RN 23124-18-7 CAPLUS
CN 9H-Purine-9-butanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16



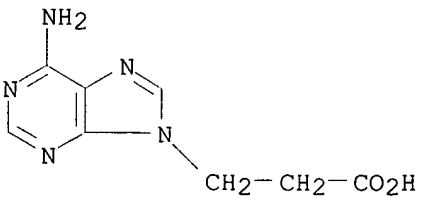
RN 25477-96-7 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 88 OF 116 CAPLUS COPYRIGHT 2002 ACS
1985:39817 Document No. 102:39817 The crystal structure of 3-(adenin-9-yl)-N-(2-succinimidyl)propionamide and hydrogen bonding scheme of anticonvulsant drugs with adenine. Takimoto, Midori; Takenaka, Akio; Sasada, Yoshio (Lab. Chem. Nat. Prod., Tokyo Inst. Technol., Yokohama, 227, Japan). Bull. Chem. Soc. Jpn., 57(11), 3070-3 (English) 1984. CODEN: BCSJA8. ISSN: 0009-2673.

AB 3-(Adenin-9-yl)-N-(2-succinimidyl)propionamide [94129-52-9] has been synthesized as a model for studying the interaction between cyclic ureide and adenine [73-24-5], and its crystal structure examd. The crystals are monoclinic, the space group P21/c, with unit-cell dimensions of a = 10.861 (1), b = 12.766(1), c = 9.753 (1) .ANG., .beta. = 91.10(1).degree., and Z = 4. The ureide moiety is hydrogen bonded to adenine with NH...N(1) (2.903(3) .ANG.) and O...HN(6) (2.955(3) .ANG.). A comparison of the hydrogen bonding patterns of the related compds. with adenine suggests that cyclic ureide anticonvulsant drugs possess the capability of interacting with N(1) and N(6) sites of adenine.

IT **4244-47-7**
RL: BIOL (Biological study)
(condensation of, with asparagine Me ester HCl)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 89 OF 116 CAPLUS COPYRIGHT 2002 ACS
1983:571467 Document No. 99:171467 Synthesis and properties of poly(amino acids) containing pendant nucleic acid bases. Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Proc. IUPAC, I. U. P. A. C.,

Searched by: Mary Hale 308-4258 CM-1 12D16

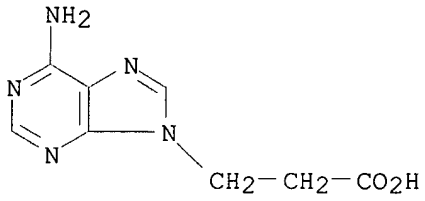
Macromol. Symp., 28th, 375. Int. Union Pure Appl. Chem.: Oxford, UK. (English) 1982. CODEN: 50DXAF.

AB Poly-L-lysine contg. pendant nucleic acid bases (adenine, thymine, uracil, or theophylline) were prepd., and their conformations and interactions were studied.

IT **4244-47-7**
RL: RCT (Reactant)
(reaction of, with polylysine)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 90 OF 116 CAPLUS COPYRIGHT 2002 ACS

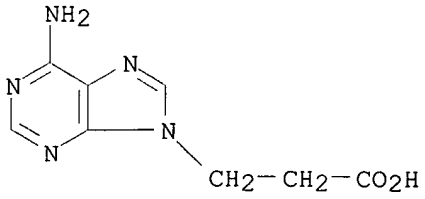
1983:54640 Document No. 98:54640 Functional monomers and polymers. CII. Synthesis and properties of oligomer models of polyethyleneimine derivatives containing pendant adenine bases. Sakuma, Yo; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, Japan). J. Polym. Sci., Polym. Chem. Ed., 20(12), 3431-46 (English) 1982. CODEN: JPLCAT. ISSN: 0449-296X.

AB A series of oligomeric model compds. of polyethylenimine derivs. with pendant adenine bases were prepd. by the reaction of a carboxyethyl deriv. of adenine with oligomeric amines, using an activated ester method. To evaluate the intramol. interaction between pendant adenine bases in these compds., UV spectra at various pH regions were measured. UV hypochromicities and pK.alpha. values depended linearly on the chain length of the oligomers. The intramol. interactions of adenine bases were fewer in their protonated forms than in their neutral forms.

IT **4244-47-7**
RL: RCT (Reactant)
(reaction of, with dicyclohexylamine)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



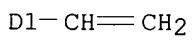
L27 ANSWER 91 OF 116 CAPLUS COPYRIGHT 2002 ACS

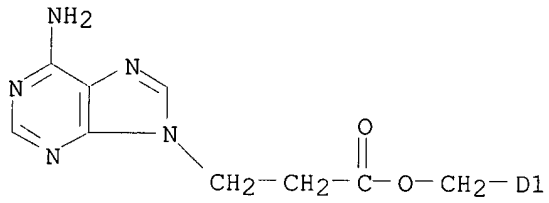
1982:563584 Document No. 97:163584 Spacer effect in the template polycondensation of nucleotide analogs with diamines. Nakagawa, Hiroshi; Muraki, Michiro; Miura, Yozo; Kinoshita, Masayoshi (Fac. Eng., Osaka City Univ., Osaka, Japan). Makromol. Chem., 183(9), 2065-70 (English) 1982. CODEN: MACEAK. ISSN: 0025-116X.

AB The template effect of polystyrene contg. 3-(9-adenylpropionyl)oxymethyl group bounded via a styrene spacer group. on the polycondensation of

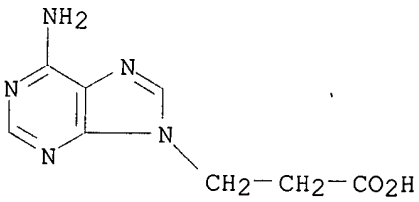
active esters [bis(p-nitrophenyl) 2-(thymin-1-ylmethyl)succinate (I) and bis(2-nitrophenyl) 2-(theophyllin-7-ylmethyl)succinate (II)] with diamines was studied in pyridine-CH_2Cl_2 or DMF. Template polymers accelerated the polycondensation of I with diamines by a factor of 5-20, but the polycondensation of II with piperazine showed no appreciable template effect.

IT **83372-27-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 83372-27-4 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino-, (ethenylphenyl)methyl ester (9CI) (CA INDEX NAME)



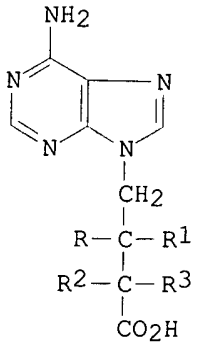


IT **4244-47-7**
RL: USES (Uses)
(vinylbenzylation of)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)

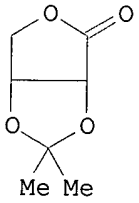


L27 ANSWER 92 OF 116 CAPLUS COPYRIGHT 2002 ACS
1982:563390 Document No. 97:163390 Studies on S-adenosyl-L-homocysteine hydrolase. Part V. Synthesis and antiviral activity of stereoisomeric eritadenines. Holy, Antonin; Votruba, Ivan; De Clercq, Erik (Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10/6, Czech.). Collect. Czech. Chem. Commun., 47(5), 1392-407 (English) 1982. CODEN: CCCCAK. ISSN: 0366-547X.
GI

Searched by: Mary Hale 308-4258 CM-1 12D16



I, R=R2=OH, R1=R3=H
II, R=R2=H, R1=R3=OH
III, R=R3=H, R1=R2=OH
IV, R=R3=OH, R1=R2=H

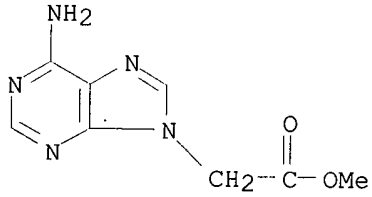


V

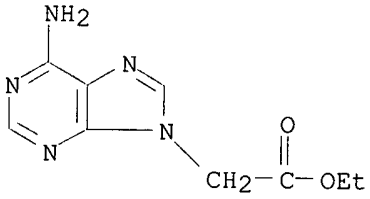
AB Stereoisomeric eritadenines I-IV were prepd. by various methods, e.g., erythronolactone V was treated with adenine in Me2SO in the presence of K2CO3, the product was deprotected by acid hydrolysis and then chromatographed on Dowex 50 .times. 8 (H+ form) column to give 30% I. I and II were active against vaccinia, measles, and vesicular stomatitis virus; I was also effective against reo- and parainfluenza virus. In general the antiviral activity decreased in the order I > II .mchgt. III, IV.

IT **23124-10-9P 25477-96-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 23124-10-9 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, methyl ester (8CI, 9CI) (CA INDEX NAME)



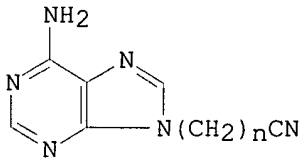
RN 25477-96-7 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



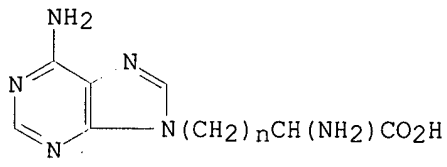
L27 ANSWER 93 OF 116 CAPLUS COPYRIGHT 2002 ACS
1982:423519 Document No. 97:23519 Formation of (adenin-9-yl)-.omega.-cyanoalkanes from (adenin-9-yl)-.alpha.-amino acids. Poritere, S.; Paegle, R.; Lidaks, M. (Inst. Org. Sint., Riga, 226006, USSR). Khim. Geterotsikl. Soedin. (4), 539-41 (Russian) 1982. CODEN: KGSSAQ. ISSN: 0453-8234.

GI

Searched by: Mary Hale 308-4258 CM-1 12D16



I



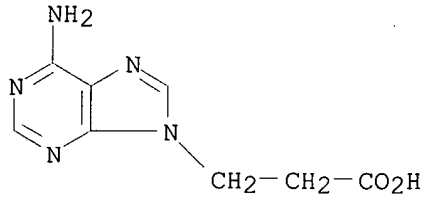
II

AB The title compds. I (n = 1-4) were prepd. in 63-86% yields by treatment of II (n as above) with Br in an acetate buffer at 20.degree..

IT **4244-47-7**
RL: RCT (Reactant)
(bromination of)

RN 4244-47-7 CAPLUS

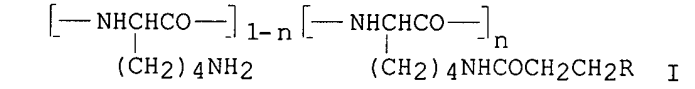
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



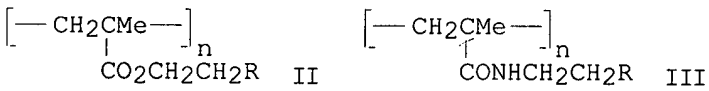
L27 ANSWER 94 OF 116 CAPLUS COPYRIGHT 2002 ACS

1981:47875 Document No. 94:47875 Functional monomers and polymers. LXXXIV. On the specific base-base interaction between polymers having complementary nucleic acid bases. Inaki, Yoshiaki; Ishikawa, Tomohiro; Sugita, Shinichi; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Osaka, Japan). J. Polym. Sci., Polym. Lett. Ed., 18(11), 725-36 (English) 1980. CODEN: JPYBAN. ISSN: 0360-6384.

GI



I



II III

AB Formation of polymer complexes between poly-L-lysine derivs. (I; R = adenin-9-yl, thymin-1-yl, uracil-1-yl) and polymethacrylates (II; R = adenin-9-yl, thymin-1-yl) or polymethacrylamides (III; R = adenin-9-yl, uracil-1-yl) was studied. High-mol.-wt. I contg. 93 mol % nucleic acid base formed stable complexes with II (R = adenin-9-yl)(IV) [25750-76-9] or II (R = adenin-1-yl) [76287-73-5] by stoichiometric 1:1 interaction resulting from specific pendant base pairing, and the structure of the complexes was assumed to be helical. However, low-mol.-wt. I, having a random coil structure, did not form stable complexes with IV. The value of hypochromicity decreased markedly with thymine content in I; e.g., I (R = thymin-1-yl)(V) contg. 65 mol % thymine formed a 5:1 complex with IV which did not agree with the theor. stoichiometry of the binding sites

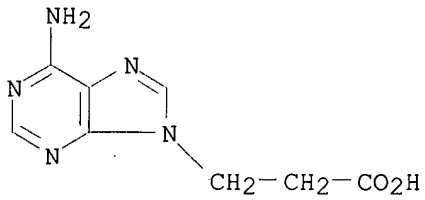
Searched by: Mary Hale 308-4258 CM-1 12D16

(2:3), presumably because of the inability of the random coil part of V to form a stable polymer complex. III also formed stable complexes with low-mol.-wt. I whereas II did not, and the difference was attributed to the higher chain penetration ability of III.

IT **4244-47-7D**, reaction products with poly-L-lysine
RL: PRP (Properties)
(interaction of, with nucleic acid base-modified methacrylic polymers)

RN 4244-47-7 CAPLUS

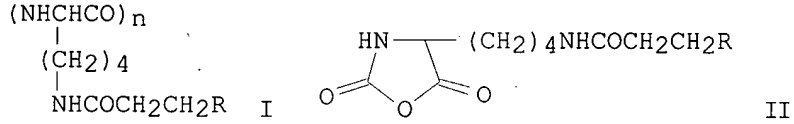
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 95 OF 116 CAPLUS COPYRIGHT 2002 ACS

1981:16046 Document No. 94:16046 Synthesis of poly-L-lysine containing nucleic acid bases. Inaki, Y.; Ishikawa, T.; Tayemoto, K. (Fac. Eng., Osaka Univ., Suita, 565, Japan). ACS Symp. Ser., 121(Modif.`Polym.), 359-70 (English) 1980. CODEN: ACSMC8. ISSN: 0097-6156.

GI

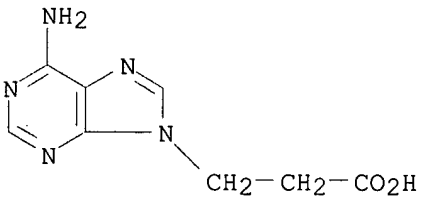


AB Polylysine was condensed with RCH2CH2CO2C6H4NO2-p (R = adenine moiety, thymine moiety, uracil moiety) to give N.epsilon.-substituted polylysines I. I were also prepd. by the polymn. of carboxyanhydrides II. Poly(glutamic acids) contg. pendant nucleic acid bases were also prepd. by the polymn. of the corresponding N-carboxyanhydrides.

IT **4244-47-7DP**, .epsilon.-amide with polylysine
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR of)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 96 OF 116 CAPLUS COPYRIGHT 2002 ACS

1980:586709 Document No. 93:186709 Functional monomers and polymers. Part LXVII. Synthesis of nucleic base-containing chitosan derivatives. Sakuma, Yo; Inaki, Yoshiaki; Takemoto, Kiichi (Dep. Petrochem., Osaka

Searched by: Mary Hale 308-4258 CM-1 12D16

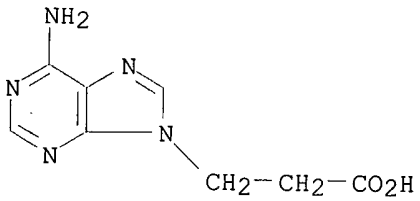
Univ., Osaka, Japan). Technol. Rep. Osaka Univ., 30(1517-1550), 319-23 (German) 1980. CODEN: TROUAI. ISSN: 0030-6177.

AB The nucleoside bases uracil, theophylline, and adenine were incorporated in vinylamine-vinyl alc. copolymer and chitosan via the pentachlorophenyl esters of their carboxyethyl derivs. The rate of incorporation of the bases in the copolymer was 58-81% and in chitosan 5-50%.

IT **4244-47-7**
RL: RCT (Reactant)
(esterification of)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 97 OF 116 CAPLUS COPYRIGHT 2002 ACS

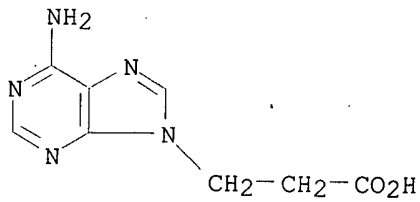
1979:457766 Document No. 91:57766 Graft copolymers containing nucleic acid bases and L-.alpha.-amino acids. Overberger, C. G.; Inaki, Yoshiaki (Dep. Chem., Univ. Michigan, Ann Arbor, MI, 48109, USA). J. Polym. Sci., Polym. Chem. Ed., 17(6), 1739-58 (English) 1979. CODEN: JPLCAT. ISSN: 0449-296X.

AB Nitrophenyl esters of (carboxyethyl)adenine (I) and (carboxyethyl)thymine (II) were grafted on linear and branched poly(ethylenimine) (III), and amino acids (alanine, aspartic acid, serine, and histidine) were grafted on linear III. The amino acid-linear III reaction products were condensed with nitrophenyl esters of I and II.

IT **4244-47-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 98 OF 116 CAPLUS COPYRIGHT 2002 ACS

1979:420943 Document No. 91:20943 Synthesis of new mono- and disubstituted hydroxyalkyl and aminoalkyl derivatives of heterocyclic bases. Holy, Antonin (Inst. Org. Chem. Biochem., Czechoslovak Acad. Sci., Prague, Czech.). Collect. Czech. Chem. Commun., 43(12), 3444-65 (English) 1978. CODEN: CCCCAK. ISSN: 0366-547X.

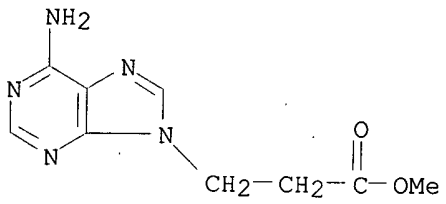
AB Adenine derivs. contg. an aliph. chain with 1 or 2 OH, NH2, or OMe groups and also some derivs. of the corresponding carboxylic acids were prepd. Several analogs contg. other heterocycles were also prepd. The compds. were prepd. for screening for antibacterial and antiviral activities; none of the compds. were inhibitory against Escherichia coli at concns. up to

1000 .mu.g/mL (results of antiviral screening not given). Thus, reaction of adenine with Me acrylate gave 3-(adenin-9-yl)- (I) and 3-(adenin-3-yl)propionic acid. Esterification of I with CH2N2 and redn. of the ester with NaBH4 gave 9-(3-hydroxypropyl)adenine.

IT **70259-15-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydride redn. of)

RN 70259-15-3 CAPLUS

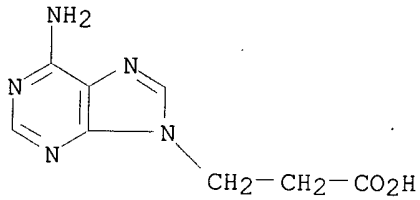
CN 9H-Purine-9-propanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)



IT **4244-47-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and methylation of)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 99 OF 116 CAPLUS COPYRIGHT 2002 ACS

1977:182968 Document No. 86:182968 Inhibitors of hypoxanthine metabolism in Ehrlich ascites tumor cells in vitro. Smith, Camilla M.; Zombor, George; Henderson, J. Frank (Cancer Res. Unit, Univ. Alberta, Edmonton, Alberta, Can.). Cancer Treat. Rep., 60(10), 1567-84 (English) 1976. CODEN: CTRRDO.

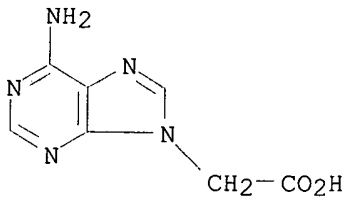
AB One hundred and sixty-one purine analogs and derivs. were tested for their ability to inhibit ten parameters of purine [120-73-0] metab. in Ehrlich ascites tumor cells incubated in vitro with radioactive hypoxanthine. Sixty-seven compds. were inhibitory against at least one parameter and 30 were inhibitory against two or more.

IT **20128-29-4**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(purine metab. by neoplasm response to)

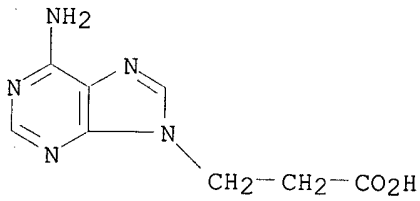
RN 20128-29-4 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)

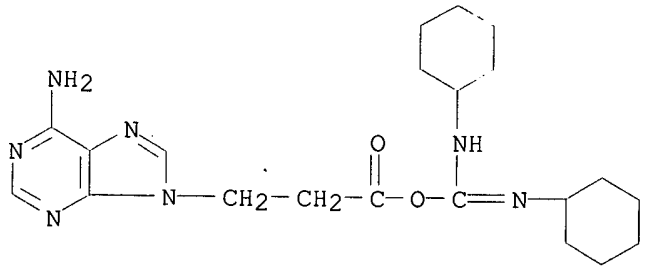
Searched by: Mary Hale 308-4258 CM-1 12D16



L27 ANSWER 100 OF 116 CAPLUS COPYRIGHT 2002 ACS
1976:60038 Document No. 84:60038 Functional monomers and polymers. 28. Synthesis and polymerization of nucleic-base containing styrene derivatives. Kondo, Koichi; Sato, Toshiaki; Inaki, Yoshiaki; Takemoto, Kiichi (Tech. Fac., Univ. Osaka, Suita, Japan). Makromol. Chem., 176(11), 3505-9 (German) 1975. CODEN: MACEAK.
GI For diagram(s), see printed CA Issue.
AB The reaction of uracil [66-22-8], thymine [65-71-4], or theophylline [58-55-9] with propiolactone (I) [57-57-8] and 4-aminostyrene (II) [1520-21-4] gave compound III [57992-45-7] and analogous thymine and theophylline derivs. which were homopolymd. or copolymd. with styrene in the presence of AIBN. The reaction of adenine [73-24-5] with I and II gave 9-[3-oxo-3-(4-vinylanilino)-1-propyl]adenine polymer [57998-20-6].
IT **4244-47-7P 57992-44-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



RN 57992-44-6 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino-, anhydride with N,N'-dicyclohexylcarbamimidic acid (9CI) (CA INDEX NAME)



L27 ANSWER 101 OF 116 CAPLUS COPYRIGHT 2002 ACS
1975:140428 Document No. 82:140428 Oxidation of reversed nucleosides in oxygen. IV. Synthesis of 4-(6-aminopurine-9H-9-yl)-3(R)-hydroxy-2(R)-aminobutyric acid. Kanno, Takeshi; Kawazu, Mitsutaka (Org. Chem. Res.

Searched by: Mary Hale 308-4258 CM-1 12D16

Lab., Tanabe Seiyaku Co., Ltd., Toda, Japan). Chem. Pharm. Bull., 22(12), 2851-60 (English) 1974. CODEN: CPBTAL.

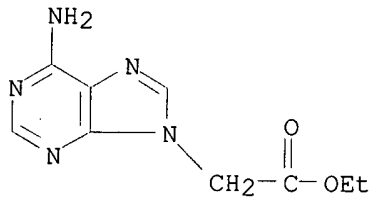
GI For diagram(s), see printed CA Issue.

AB Treatment of 5-O-tosyl-3-benzyloxycarbonylamido- or 5-O-tosyl-3-acetamido-3-deoxy-1,2-O-isopropylidene-.alpha.-D-ribofuranose with the Na salt of adenine afforded the corresponding isomeric reversed nucleosides. Hydrolysis of I (R1R1 = Me2C, R2 = PhCH2O2C) followed by hydrogenolysis gave I.HCl (R1 = R2 = H). After deblocking, oxidn. of I (R1 = H, R2 = Ac) by O in a dil. alk. soln. afforded Na 4-(6-aminopurin-9H-9-yl)-3(R)-hydroxy-2(R)-acetamidobutyrate.

IT **25477-96-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 102 OF 116 CAPLUS COPYRIGHT 2002 ACS

1975:140427 Document No. 82:140427 Oxidation of reversed nucleosides in oxygen. III. Synthesis of eritadenine analogs of purines and pyrimidines. Kanno, Takeshi; Kawazu, Mitsutaka (Org. Chem. Res. Lab., Tanabe Seiyaku Co., Ltd., Toda, Japan). Chem. Pharm. Bull., 22(12), 2836-50 (English) 1974. CODEN: CPBTAL.

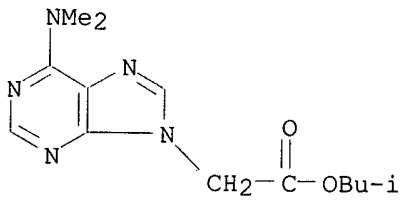
GI For diagram(s), see printed CA Issue.

AB Reaction of Me 5-O-tosyl-2,3-O-isopropylidene-.beta.-D-ribofuranoside with the Na salts of purines and pyrimidines in DMF afforded the corresponding reversed nucleosides. 6-Alkylaminopurine analogs I (R = NHBu, NMe2, furfurylamino) were prepd. by the reaction of I (R = SMe) with amines. After deblocking, the reversed nucleosides were oxidized by O in dil. alk. soln. to afford eritadenine analogs.

IT **55175-42-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 55175-42-3 CAPLUS

CN 9H-Purine-9-acetic acid, 6-(dimethylamino)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 103 OF 116 CAPLUS COPYRIGHT 2002 ACS

1975:25663 Document No. 82:25663 Synthesis and hypocholesterolemic activities of eritadenine derivatives. Okumura, Kentaro; Matsumoto, Kazuo; Fukamizu, Masaharu; Yasuo, Harunori; Taguchi, Yoshihiko; Sugihara,

Yukio; Inoue, Ichizo; Seto, Masahiko; Sato, Yasuhiko; et al. (Res. Lab., Tanabe Seiyaku Co., Ltd., Toda, Japan). J. Med. Chem., 17(8), 846-55 (English) 1974. CODEN: JMCMAR.

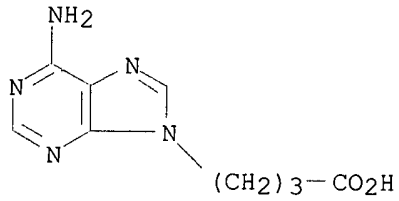
GI For diagram(s), see printed CA Issue.

AB More than 100 title compds. were prepd. by esterification or amidation of eritadenine (I) [23918-98-1], alkylation of adenine [73-24-5] with O-protected 2(R),3(R)-Et 4-bromo-2,3-dihydroxybutyrate [53186-35-9], or ring closure of appropriate aminocyanoimidazolylribonucleosides followed by hydrolysis and oxidn. In tests in rats for hypocholesterolemic activity, esters of I with short chain alcs. were 25 to 50 times as active as I, with a minimal effective dose in diet as low as 0.1 mg/kg/day. I is about 10 times as active as clofibrate [637-07-0]. Structure-activity relations were discussed.

IT **33147-28-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and anticholesteremic activity of)

RN 33147-28-3 CAPLUS

CN 9H-Purine-9-butanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 104 OF 116 CAPLUS COPYRIGHT 2002 ACS

1975:327 Document No. 82:327 Hypocholesterolemic activity of analogous compounds related to eritadenine, and active component of Shiitake, Lentinus edodes. Tensho, Akira; Shimizu, Iwao; Takenawa, Tadaomi; Kikuchi, Hiroyuki; Rokujo, Tsuneshige; Kamiya, Takashi (Res. Lab., Fujisawa Pharm. Co., Ltd., Tokyo, Japan). Yakugaku Zasshi, 94(6), 708-16 (Japanese) 1974. CODEN: YKKZAJ.

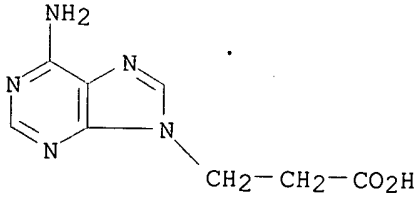
GI For diagram(s), see printed CA Issue.

AB Eritadenine (I) [23918-98-1] esters given orally to rats were 10 times as active as I itself in serum cholesterol-lowering activity. The activity required the presence of purine ring in the mols. and of NH2 or similar basic substituents at the 6 position. As to the side chain of I, the presence of butyric acid with OH at .alpha. or .beta. position induced a strong activity. The activities of 66 I derivs. were studied.

IT **4244-47-7 33147-28-3**
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anticholesteremic activity of)

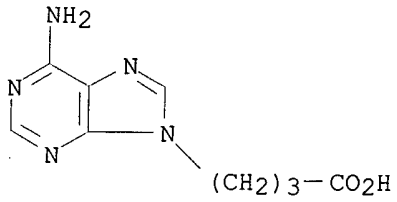
RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



Searched by: Mary Hale 308-4258 CM-1 12D16

RN 33147-28-3 CAPLUS
CN 9H-Purine-9-butanoic acid, 6-amino- (9CI) (CA INDEX NAME)

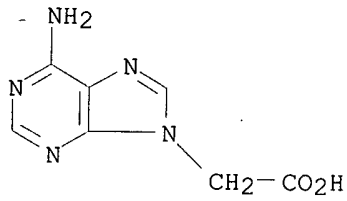


L27 ANSWER 105 OF 116 CAPLUS COPYRIGHT 2002 ACS
1973:537090 Document No. 79:137090 Synthesis of carboxymethyl derivatives of purines and pyrimidines and their condensation with naturally occurring macromolecules. Jones, A. S.; Lewis, P.; Withers, S. F. (Chem. Dep., Univ. Birmingham, Birmingham, Engl.). Tetrahedron, 29(15), 2293-6 (English) 1973. CODEN: TETRAB.

AB 1-(Carboxymethyl)thymine (I), 1-(carboxymethyl)cytosine, and 9-(carboxymethyl)adenine (II) were prepd. from the appropriate bases and a Na haloacetate in alkali. Deamination of II with HNO2 gave 9-(carboxymethyl)hypoxanthine (III). 1-(Carboxymethyl)uracil, I, and III were condensed with protamine and dextran to give H2O-sol., base-substituted polymers. I-dextran showed a slow decrease in optical d. at 268 nm in 2 .times. SCC (SCC = 0.015M Na citrate, 0.015M NaCl) at 20.degree. of 30%. No decrease occurred in 7M urea. I-dextran gave an addnl. hypochromic effect with polyadenylic acid in 2 .times. SCC at 4.degree. and 14.degree. of 13 and 9% resp. The thymine-adenine residue ratio at max. hypochromicity was 3:1.

IT **20128-29-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 20128-29-4 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 106 OF 116 CAPLUS COPYRIGHT 2002 ACS
1973:479105 Document No. 79:79105 Oxidation of "reversed nucleosides" in oxygen. I. Synthesis of eritadenine and its derivatives. Kawazu, Mitsutaka; Kanno, Takeshi; Yamamura, Shiro; Mizoguchi, Tomishige; Saito, Seiichi (Org. Chem. Res. Lab., Tanabe Seiyaku Co. Ltd., Toda, Japan). J. Org. Chem., 38(16), 2887-90 (English) 1973. CODEN: JOCEAH.

AB Reaction of Me 5-O-tosyl-2,3-O-isopropylidene-.beta.-D-ribofuranoside or 5-O-tosyl-1,2-O-isopropylidene-3-O-alkyl-.beta.-D-arabinofuranoses with the Na salt of adenine in DMF afforded good yields of the corresponding reversed nucleosides. After removal of the protective groups from the sugar moiety by treatment with HCl, the deblocked reversed nucleosides were oxidized by air or oxygen in a dilute alkali soln. at room temp. to give eritadenine and its .alpha.-O-alkyl derivs. in good yields.

Searched by: Mary Hale 308-4258 CM-1 12D16

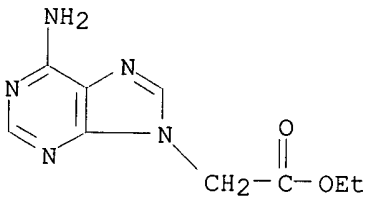
Esterification confirmed the structures and the biological activities were evaluated.

IT **25477-96-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 107 OF 116 CAPLUS COPYRIGHT 2002 ACS

1973:442452 Document No. 79:42452 Synthetic spectroscopic models related to coenzymes and base pairs. XII. Controlled interaction between nucleic acid bases. Intramolecular stacking interactions between two adenine rings. Leonard, Nelson J.; Ito, Keiichi (Sch. Chem. Sci., Univ. Illinois, Urbana, Ill., USA). J. Amer. Chem. Soc., 95(12), 4010-16 (English) 1973. CODEN: JACSAT.

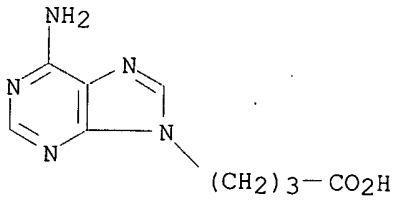
AB To det. the stacking interactions between two parallel rings oriented at different axis angles toward each other, a series of six different trimethylenebisadenine isomers was synthesized. The per cent hypochromism, H, for the long wavelength uv absorption band for each of these compds was detd. by comparison of the uv spectrum of the trimethylenebisadenine in aq. soln. with the composite spectrum of the two half mol., the appropriate propyladenines. The H values obtained thereby for the trimethylenebisadenines are the following: 9,9'isomer, 15%; N6,N6', 16%; 8,8', 21%; N6,9', 16%; 8,9', 19%; 7,9', 16%. The per cent hypochromism follows a dependence upon the folded confor- mations available to the individual trimethylenebisadenines and offers the possiblity of assessing the degree and orientation of overlap per- mitted or excluded for different ranges of H values.

IT **33147-28-3P 41785-06-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 33147-28-3 CAPLUS

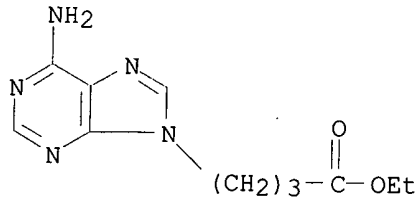
CN 9H-Purine-9-butanoic acid, 6-amino- (9CI) (CA INDEX NAME)



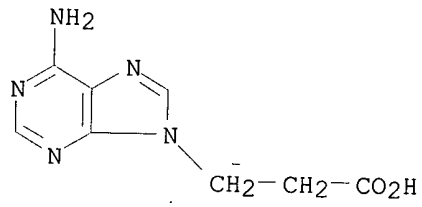
RN 41785-06-2 CAPLUS

CN 9H-Purine-9-butanoic acid, 6-amino-, ethyl ester (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16



L27 ANSWER 108 OF 116 CAPLUS COPYRIGHT 2002 ACS
1973:84435 Document No. 78:84435 9-Carboxyethyladenine polycondensates. Takemoto, Kiichi; Kondo, Koichi (Chisso Co., Ltd.). Jpn. Kokai Tokkyo Koho JP 47033196 19721117 Showa, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1971-13921 19710315.
GI For diagram(s), see printed CA Issue.
AB Acid halides of 9-carboxyethyladenine were polycondensed to give the title compds. (I) useful as intermediates for pharmaceuticals and agricultural chemicals. Thus, 0.5 g 9-(carboxyethyl)adenine, 0.5 g PCl5, and 3 ml AcCl was reacted for 24 hr at room temp. and the reaction products washed with petroleum ether and stirred for 1 week at room temp. with 100 ml DMF and 10 ml Et3N to give 0.047 g I, d.p. 2-5.
IT **4244-47-7**
RL: RCT (Reactant)
(reaction of, with phosphorus pentachloride and acetyl chloride)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 109 OF 116 CAPLUS COPYRIGHT 2002 ACS
1973:58470 Document No. 78:58470 N-Carboxyethylpurine derivatives. Takemoto, Kiichi; Kondo, Koichi (Chisso Co., Ltd.). Jpn. Kokai Tokkyo Koho JP 47030694 19721109 Showa, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1971-13920 19710313.
AB Purine derivs. having no substituent at 7- or 9-position was treated with .beta.-propiolactone (I). E.g., Adenine, I, and small amt. of NaOH in DMF was refluxed 2 hr to give 43% 9-(2-carboxyethyl)adenine. Similarly prepd. was 7-(2-carboxyethyl)theophylline.
IT **4244-47-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)

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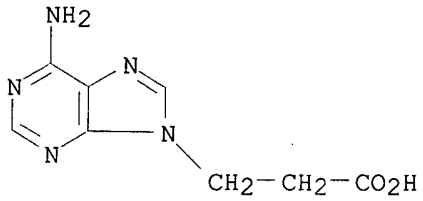
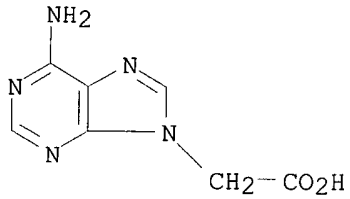
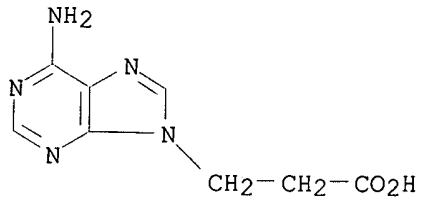


L27 ANSWER 110 OF 116 CAPLUS COPYRIGHT 2002 ACS
1973:29824 Document No. 78:29824 9-Carboxymethyladenine. Takemoto, Kiichi; Kondo, Koichi (Chisso Co., Ltd.). Jpn. Kokai Tokkyo Koho JP 47030696 19721109 Showa, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1971-13923 19710313.
GI For diagram(s), see printed CA Issue.
AB The title compd. (I) was prepd. by hydrolysis and decarboxylation of dialkyl 9-adenylmalonate. E.g., 1.4 g di-Et 9-adenylmalonate in EtOH-H2O (1:3) was stirred 3 days with 0.3 g NaOH to give 0.15 g I.
IT **20128-29-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 20128-29-4 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)

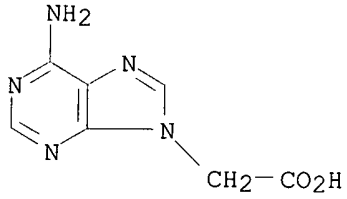


L27 ANSWER 111 OF 116 CAPLUS COPYRIGHT 2002 ACS
1972:3801 Document No. 76:3801 Synthesis of carboxylic acid derivatives of adenine and theophylline. Kondo, Koichi; Miyata, Mikiji; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, Japan). Bull. Chem. Soc. Jap., 44(9), 2554-5 (English) 1971. CODEN: BCSJA8.
GI For diagram(s), see printed CA Issue.
AB Treatment of adenine (I) with NaH and then BrCH(CO2Et)2 in DMF gave di-Et adenine-9-malonate, [II, R = CH(CO2Et)2], which was sapond. to give II [R = CH(CO2H)2, CH2CO2H]. Theophylline and I reacted with .beta.-propiolactone in DMF in the presence of base to give 7-(.beta.-carboxyethyl)theophylline and II (R = CH2CH2CO2H), resp. Treatment of the latter with PCl5 and then Et3N in DMF yielded a polyamide of probable structure III.
IT **4244-47-7P 20128-29-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)

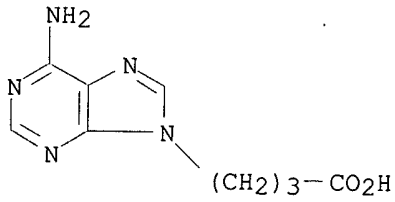
Searched by: Mary Hale 308-4258 CM-1 12D16



RN 20128-29-4 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 112 OF 116 CAPLUS COPYRIGHT 2002 ACS
1971:463742 Document No. 75:63742 Novel carboxyalkylations of purines by .gamma.-lactones. De Kock, D. H.; Raubenheimer, H. G. (Dep. Chem., Univ. Stellenbosch, Stellenbosch, S. Afr.). J. S. Afr. Chem. Inst., 24(May), 91-5 (English) 1971. CODEN: JSACAT.
GI For diagram(s), see printed CA Issue.
AB 4-(N3-Adenyl)butyric acid (I) and 4-(N7-guanyl)butyric acid (II) are prepd. by the reaction of purines with .gamma.-butyrolactone (III). Thus, a mixt. of adenine and III is refluxed to give 4-(N9-adenyl)butyric acid (IV) and I (major product). Guanine gives 4-(N9-guanyl)butyric acid (V) and II (major product). Adenosine is treated with III to gibe I and IV, and II and V are obtained from guanosine. A mixt. of adenylic acid, III, and water is kept at 40.degree. to give IV.
IT **33147-28-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 33147-28-3 CAPLUS
CN 9H-Purine-9-butanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 113 OF 116 CAPLUS COPYRIGHT 2002 ACS
1971:84028 Document No. 74:84028 Two new constituents from Lentinus edodes. Saito, Yoshihisa; Hashimoto, Masashi; Seki, Hideo; Kamiya, Takashi (Res. Lab., Fujisawa Pharm. Co. Ltd., Osaka, Japan). Tetrahedron Lett. (56), 4863-6 (English) 1970. CODEN: TELEAY.
GI For diagram(s), see printed CA Issue.
AB 4(6Amino9HPurin99yl)2(R)Hydroxybutyric acid (deoxyeritadennd 3(69amino9HPurin9Yl)propionic acid [I, R = CH(OH)CO2D CO2H resp.] were

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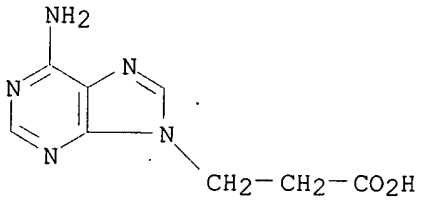
isolated from L. edodes. Their structures were confirmed by synthesis.

IT **4244-47-7**
RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)
(of Lentinus edodes)

RN 4244-47-7 CAPLUS

CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



L27 ANSWER 114 OF 116 CAPLUS COPYRIGHT 2002 ACS

1970:43617 Document No. 72:43617 Decarboxylation of some carboxymethyladenines. Lira, Emil P. (Growth Sci. Center, Intern. Miner. and Chem. Corp., Libertyville, Ill., USA). J. Heterocycl. Chem., 6(6), 955-7 (English) 1969. CODEN: JHTCAD.

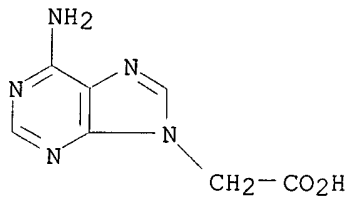
GI For diagram(s), see printed CA Issue.

AB 3-Ethoxycarbonylmethyladenine and 9-ethoxy-carbonylmethyladenine were acid-hydrolyzed to 3-carboxymeth-yladenine (I) and 9-carboxymethyladenine (II), resp. I was decarboxylated at 300-5.degree./0.4 mm to 3-methyladenine. Under the same conditions most of the II had sublimed by the time the reaction temp. was reached, but the remaining II was not decarboxylated. The difference in reactivity between I and II was explained by their di fferent basicities. The pKa of the Et esters of I and II were 6.4 and 3.7, resp.

IT **20128-29-4P 25477-96-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

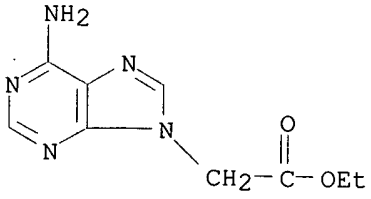
RN 20128-29-4 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



RN 25477-96-7 CAPLUS

CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



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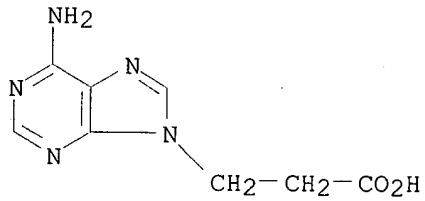
L27 ANSWER 115 OF 116 CAPLUS COPYRIGHT 2002 ACS
1969:449898 Document No. 71:49898 Syntheses of some 9-substituted adenines as inhibitors of adenosine deaminase. Chakraborti, S. K. (Chittaranjan Nat. Cancer Res. Centre, Calcutta, India). Indian J. Chem., 7(5), 426-9 (English) 1969. CODEN: IJOCAP.

GI For diagram(s), see printed CA Issue.

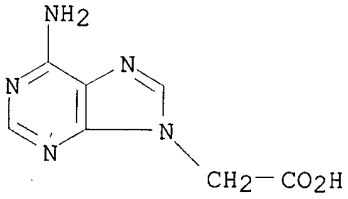
AB The syntheses of some adenines (I) (n = 1-3, R = CO2H, CO2Me, CN, NH2, CH2NH2, CO2C6H4NO2-p), as possible inhibitors of adenosine deaminase are described. Most of the compds. are either weakly inhibitory or non-inhibitory to adenosine deaminase.

IT **4244-47-7P 20128-29-4P 23124-10-9P 23124-18-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

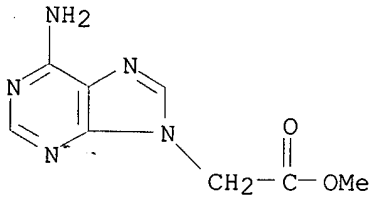
RN 4244-47-7 CAPLUS
CN 9H-Purine-9-propanoic acid, 6-amino- (9CI) (CA INDEX NAME)



RN 20128-29-4 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



RN 23124-10-9 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, methyl ester (8CI, 9CI) (CA INDEX NAME)



RN 23124-18-7 CAPLUS
CN 9H-Purine-9-butanoic acid, 6-amino-, methyl ester (9CI) (CA INDEX NAME)

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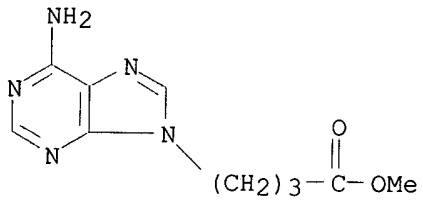
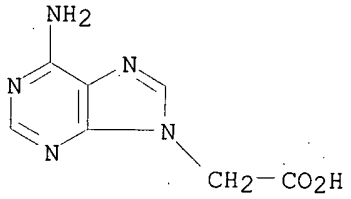


L27 ANSWER 116 OF 116 CAPLUS COPYRIGHT 2002 ACS
1968:506669 Document No. 69:106669 The action of alkali on some 9-substituted adenines. Mian, A. M.; Walker, R. T. (Univ. Birmingham, Birmingham, Engl.). J. Chem. Soc., C (20), 2577-9 (English) 1968. CODEN: JSOOAX.

AB The action of alkali on some 9-alkyladenines was shown to be of 2 types: (a) replacement of -NH2 by -OH, and (b) opening of the imidazole ring to give finally a 4,5-diamino-6-alkylaminopyrimidine. The only compd. tested which was stable was 9-carboxymethyladenine; all the other compds. gave some of the corresponding 9-alkylhypoxanthine. An approx. correlation between the amt. of 4,5-diamino-6-alkylaminopyrimidine and the Ka of the corresponding alkylcarboxylic acid is given.

IT **20128-29-4**
RL: RCT (Reactant)
(reaction of, with alkali)

RN 20128-29-4 CAPLUS
CN 9H-Purine-9-acetic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	466.42	1456.30

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-65.67	-82.19

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L28 4 L26

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L28 ANSWER 1 OF 4 CAOLD COPYRIGHT 2002 ACS
AN CA65:7178h CAOLD
TI Michael-type reactions with adenine
AU Lira, Emil P.; Huffman, C. W.
IT 711-64-8 **4244-47-7** 7051-59-4 7051-64-1 7051-65-2
7083-40-1 92503-72-5 94626-13-8

L28 ANSWER 2 OF 4 CAOLD COPYRIGHT 2002 ACS
AN CA63:18872g CAOLD
TI nonclassical antimetabolites - (XXII) simulation of 5'-phosphoribosyl binding (5) inhibition of succino-adenylate kinosynthetase by 6-mercapto-9-purinyl alkanoic acid derivs. of 4- and 5-aminosalicylic acid
AU Baker, Bernard R.; Tanna, P. M.
IT 2545-91-7 2646-81-3 3275-78-3 4323-00-6 4323-01-7 4323-02-8
4323-03-9 4323-04-0 4323-05-1 4323-06-2 4323-07-3 4323-08-4
4323-09-5 4323-10-8 4323-11-9 4323-12-0 **4323-13-1**
4323-17-5 4323-18-6 4323-19-7 4369-82-8 4369-84-0 4418-13-7
5187-88-2

L28 ANSWER 3 OF 4 CAOLD COPYRIGHT 2002 ACS
AN CA63:16350g CAOLD
TI 2-(.alpha.-hydroxybenzyl)benzimidazole analogs - (I) synthesis of 8-(.alpha.-hydroxybenzyl)purines, the diaza analogs of 2-(.alpha.-hydroxybenzyl)benzimidazole
AU Haggerty, William J., Jr.; Springer, R. H.; Cheng, C. C.
IT 2260-33-5 2836-31-9 4244-40-0 4244-41-1 4244-43-3 4244-44-4
4244-45-5 **4244-47-7** 4244-49-9 4244-51-3 4244-52-4
4244-53-5 4244-54-6 4244-55-7 4244-56-8 4244-58-0 4289-23-0
4289-25-2 4301-59-1 4367-64-0 4460-07-5 4460-08-6 4460-09-7
4460-10-0 4538-20-9 34397-00-7 97317-88-9 98882-63-4 99785-41-8

L28 ANSWER 4 OF 4 CAOLD COPYRIGHT 2002 ACS
AN CA60:4402g CAOLD
TI nonclassical antimetabolites - (XIII) simulation of the 5'-phosphoribosyl moiety of 5'-adenylic acid at the enzyme level by .omega.-carboxyalkyl and aralkyl groups attached to adenine
AU Baker, Bernard R.; Sachdev, H. S.
IT 3342-88-9 17756-30-8 28492-53-7 34397-01-8 34397-05-2 82222-85-3
90794-86-8 90887-73-3 **90973-36-7** 91130-15-3 92103-05-4
92103-06-5 92150-21-5 92150-24-8 97026-04-5 97172-86-6 101176-01-6
101176-02-7 106384-24-1

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.66	1458.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION

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